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# A review of lead leakage monitoring in perovskite solar cells: emerging detection technologies, just transition to clean energy and perspectives

 Benjamin K. Korir,<sup>a</sup> Samantha Ndlovu,<sup>b</sup> Vincent O. Nyamori <sup>b</sup>  
 and Joshua K. Kibet <sup>\*a</sup>

Lead-based perovskite solar cells (LPSCs) offer promise for low-cost, highly efficient alternatives to current solar energy technologies, with the potential for scale-up production and high-throughput coating. However, lead leakage, which is considered a health hazard, instability due to moisture intrusion into the perovskite core, and degradation challenges remain unresolved. Without reliable monitoring and mitigation strategies, the scalability of LPSCs raises regulatory and environmental problems. Currently, systematic detection and quantification of lead (Pb) leakage are scarcely developed. Therefore, there is urgent need for real-time monitoring systems for better Pb leakage detection and monitoring to ensure public and environmental health protection. Accordingly, leakage of Pb into the environment has far-reaching etiological risks to animal and plant health. For instance, the bioaccumulation of Pb in the human body can exacerbate the development of cardiovascular diseases and damage to the central nervous system. This study provides a detailed overview of the approaches used to monitor leakage in perovskite solar cells (PSCs), closing the loop in Pb recycling, and the outlook for perovskite recycling. Here, we analyse Pb leakage monitoring and prevention approaches undertaken in recent years by reviewing scholarly databases. This study also explores the latest and emerging detection technologies, such as spectroscopic methods, electrochemical sensors, fluorescence assays, and *in situ* monitoring techniques. Just transition toward green energy access together with environmental sustainability has been explored in the event that LPSCs are ultimately deployed and commercialised. Further, the potential of artificial intelligence (AI) systems has been reviewed to understand leakage events associated with the degradation of LPSCs. To this end, this review not only provides up-to-date state-of-the-art research and developments in perovskite research but also provides insights into suitable Pb leakage monitoring and prevention strategies toward mechanically stable and environmentally sustainable LPSCs.

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## 1. Introduction

Increasing public awareness and justification for the adoption of solar energy by energy consumers is the primary factor in revitalising the acceptance of the photovoltaic technology.<sup>1,2</sup> Concurrently, as perovskite solar cell (PSC) technology is projected to grow, environmental safety is a major concern that must be balanced with affordability and efficiency. While solar energy offers significant reductions in environmental pollution, energy justice has emerged as an important concept that highlights equity, inclusivity and fairness in the transition to clean energy. The anticipated widespread deployment of photovoltaics raises concerns about environmental implications related to resource extraction, hazardous materials, and

end-of-life management, highlighting the need to address these issues through the lens of just transitions (JT) and equitable distributions of benefits and burdens.<sup>3</sup> Accordingly, the growing demand for renewable energy alternatives, particularly driven by their favourable ratio of efficiency and cost, has gained significant momentum in the 21st century.<sup>4</sup> However, the degradation of lead-based perovskite solar cells (LPSCs), such as methylammonium lead triiodide (MAPbI<sub>3</sub>), poses a significant challenge to solar cell stability and has unprecedented consequences for environmental and public health.<sup>5</sup> Whereas perovskite solar deployments have achieved rapid advancements in terms of efficiencies, there are issues that need to be addressed like the adoption of efficient Pb leakage monitoring strategies and methods for mitigating Pb pollution from LPSCs. Further, its commercial deployment has been hindered by its susceptibility to temperature and moisture, and more significantly, the toxicity of lead (Pb).<sup>6</sup> Currently, there is a lack of an appropriate treatment of MAPbI<sub>3</sub> to mitigate Pb pollution and to determine how this hazardous material can be

<sup>a</sup>Department of Chemistry, Egerton University, P.O. Box 536-20115, Njoro, Kenya.  
 E-mail: [jkibet@egerton.ac.ke](mailto:jkibet@egerton.ac.ke)

<sup>b</sup>School of Agriculture and Science, University of KwaZulu-Natal, Westville Campus,  
 Private Bag X54001, Durban 4000, South Africa



recovered and recycled. Different methods, including the most versatile inductive coupled plasma hyphenated with mass spectrometry (ICP-MS) or inductive coupled plasma atomic emission spectroscopy (ICP-AES), have been employed to quantify hazardous elements in environmental matrices,<sup>7</sup> including analytical techniques such as potentiometric and atomic adsorption spectroscopy.<sup>8</sup> However, ICP-MS and ICP-AES require highly trained experts and well-equipped laboratories.<sup>9</sup> Trace elements in the environment and food have also been determined using electrochemical methods, particularly voltammetry techniques.

The United Nations Sustainable Development Goal (SDG #7) highlights the global recognition and support for secure, affordable, and readily accessible renewable energy, climate action (SDG #13), and reduced inequalities (SDG #10). As the world strives to accomplish the challenge of “net zero” carbon in the context of SDGs, solar cell technologies have undergone the fastest rate of growth.<sup>10</sup> The International Renewable Energy Agency (IRENA) has predicted the dominance of photovoltaics in the coming years due to low costs and potentially high efficiencies.<sup>11</sup> Remarkably, organic–inorganic hybrid halide ( $\text{CH}_3\text{-NH}_3\text{PbX}_3$ , X = Cl, Br, I) PSCs offer promise for the advancement of photovoltaic technologies.<sup>12</sup> Perovskites exhibit solution-processability and a unique combination of optoelectronic properties that have enabled these devices to achieve efficiencies exceeding 27%.<sup>13</sup> Different from lightweight properties, perovskites are semi-transparent and/or flexible by means of appropriate designs.

The recyclability and life cycle assessment (LCA) of perovskite solar technologies are gaining momentum through sustainable technologies.<sup>14</sup> LPSCs have emerged as leading candidates in the renewable energy landscape because of their low cost, simplicity in production, and high performance. Nonetheless, the scalability of modules, operational instability, and materials toxicity, particularly Pb, pose serious challenges that directly relate to the ecological impact of long-term applications – these challenges inhibit deployment and commercial feasibility.<sup>15</sup> It has been widely reported previously that high-performing PSCs contain Pb, which is known to be toxic to plants and other living organisms.<sup>16</sup> PSC materials can be easily degraded under certain conditions and can dissolve in water,

releasing toxic Pb ions ( $\text{Pb}^{2+}$ ).<sup>17</sup> For practical integration of PSCs, addressing Pb toxicity, stability, and high efficiency is a key priority for the safe deployment of this promising technology, as summarized in Fig. 1. Accordingly, the use of efficient and stable Pb encapsulants is envisaged to control Pb leakage in perovskites through their lifespans. In this regard, industrial pioneers and researchers have explored Pb recycling and immobilisation strategies, as replacing Pb with other halides may require significant research time and extensive effort.

The need to improve the understanding of end-of-life (EoL) management, particularly on discarded or damaged modules that can leach into water and soil systems, and potentially threaten human health and ecosystems, is necessary.<sup>19</sup> The development of robust encapsulation and recycling procedures is crucial, given the adverse effects of Pb leakage from PSCs, even at low doses. It is important to understand perovskite degradation pathways since even low doses of Pb contamination exceed the regulatory threshold of safe exposure under acidic or humid conditions.<sup>20</sup> Degradation of weathered or damaged perovskite modules is especially rapid in coastal or tropical conditions, or even in high-energy conditions.<sup>21</sup> Critical analysis of reported incidents helps identify critical design flaws and inform the design and fabrication of safer device architectures, the use of Pb-absorbing interlayers, and multilayer encapsulation strategies. Concurrently, fundamental research is ongoing to understand the electronic, chemical, and physical properties of halide perovskites, and will continue to drive the future of device scalability and performance.<sup>18</sup>

Studies have shown that  $\text{MAPbI}_3$ -based devices are susceptible to degradation under tropical-humidity conditions, prompting the need for robust Pb containment protocols.<sup>14</sup> Besides thermal-based extraction methods, closed-loop recycling systems that can extract Pb through solvent-based methods in damaged Pb-based solar modules have been considered to enhance Pb recovery with minimal by-products. In the context of earlier investigations, recycling and immobilizing Pb within the perovskite structure reduces environmental risk and enables this new-generation technology to be scaled. The widespread adoption of PSCs focuses on addressing Pb leakage, its detrimental effects, and the strategies for Pb recovery and immobilization.<sup>22,23</sup> Different from earlier studies that have examined the toxicity risks of Pb leaching or degradation of PSCs through a material science lens in isolation, this study situates Pb leakage monitoring and links it to JT to clean energy. This review discusses ICP-MS as an indispensable gold standard *versus* a comparative critique of field deployable techniques, such as *in situ* spectroscopic techniques, electrochemical sensors, and fluorescence tests from descriptive analysis and practical applicability. Also, the novelty of this work lies in the emphasis on how real-time monitoring can help monitor  $\text{Pb}^{2+}$  leaching into water systems, linking demonstrated AI applications to conceptual approaches to Pb leakage monitoring, and EoL management of PSCs, which are still far less explored in the literature. The objectives of this review articles, thus, are four-fold (1) critical analysis of Pb leakage monitoring strategies in PSCs, (2) risk assessment of the hazardous Pb in PSCs and its relationship with monitoring strategies to inform the ecological and public health protection policies, (3) nuanced overview of predictive



Fig. 1 Key factors influencing the commercialisation of lead-based PSCs.<sup>18</sup>



modelling and AI in device design, degradation and recycling, and (4) situating the current  $\text{Pb}^{2+}$  leakage monitoring strategies and JT in the paradigm of clean energy.

## 2. Methodology

This review paper systematically and thematically summarizes existing evidence regarding the environmental, just transitions and technological issues of Pb-based halide PSCs. The approach involved critical examination of the state-of-the-art in terms of Pb leakage detection, degradation pathways, recycling methods, and the emergence of artificial intelligence (AI) in predictive diagnostics. Accordingly, this study integrates scholarly publications and industry developments, with a particular focus on LCA and environmental sustainability. A set of scholarly data databases (Web of Science, Scopus, IEEE Xplore, ScienceDirect, and Google Scholar) was examined to ensure sufficient coverage. Keywords used in the search strategy include, but are not limited to, “halide perovskites”, “leakage of lead”, “bioaccumulation”, “encapsulation technologies”, “life cycle assessment”, “recovery of lead”, “artificial intelligence in photovoltaics”, “end-of-life management”, and just transitions. Peer-reviewed articles, patents, and industrial reports, which commented directly on the environmental attributes and technological developments of PSCs, were eligible. Articles published between 2010 and 2025 were included in the study. Consequently, this article assesses Pb leaching mechanisms and environmental effects, bioaccumulation of Pb in water bodies and soil, and its impact on human health. This is informed by studies in toxicology and environmental evaluation, with an intention to highlight the urgency of combating Pb contamination from decommissioned or damaged LPSCs. Secondly, current encapsulation engineering and containment technologies like polymeric barrier films and ion-exchange layers are assessed, focusing on minimising Pb migration under both working and degradation conditions. Also, this study investigates Pb recovery and recycling techniques, which are differentiated by thermal, solvent-based, and closed-loop systems. LCA models indirectly measure the impact on the environment of these practices, particularly recovery performance and secondary waste minimisation optimization. The possibility of predicting leakage or degradation patterns using AI-powered systems is discussed. This overview presents sensor integration strategies and machine learning models for real-time monitoring and predictive maintenance of perovskite solar modules. Technologies and strategies are synthetically compared, performance, cost, environmental safety, and commercial viability analysed in relation to data advanced in literature. Future outlooks are identified by mapping emerging trends in Pb-free alternatives, just transitions and AI applications, and critically evaluated the weaknesses of the current approaches to be used in developing sustainable perovskite technologies.

## 3. Overview on the toxicity of lead

Unlike the immediate threat of degradation and leaching, a systemic risk of long-term environmental Pb build-up exists in perovskite modules. Studies have shown that even low concentrations of  $\text{Pb}^{2+}$  released into soil and groundwater can

be bio-accumulated in plants and aquatic organisms, which subsequently enter the food chain.<sup>18,24</sup> This raises concerns about chronic exposure in agricultural systems<sup>25</sup> where solar farms may compromise crop safety and livestock health. The persistence of Pb in the environment makes its elimination prohibitively costly and technologically challenging, highlighting the significance of novel Pb immobilisation strategies.<sup>15</sup> Even under minimal exposure, Pb is a critical concern for PSCs. The face density of Pb in a typical PSC with a 0.5  $\mu\text{m}$  can be determined using eqn (1).<sup>26</sup>

$$\rho_{\text{Pb}} = \frac{m_{\text{Pb}}}{A} = \frac{\rho_{\text{perovskite}} \times t \times w_{\text{Pb}}}{A} \quad (1)$$

Here,  $\rho_{\text{perovskite}}$ ,  $t$ ,  $w_{\text{Pb}}$ , and  $A$  is the density of the perovskite material, thickness, mass fraction of Pb and area, respectively. The Pb face density is approximately 70  $\mu\text{g cm}^{-2}$  for a standard device, and if a PSC module of 1.4  $\text{cm}^2$  is damaged, it could release Pb that potentially exceeds safe threshold blood levels in children. Another critical concern is the toxicity of Pb-based degradation by-products, such as  $\text{PbI}_2$ ,  $\text{PbO}$ , and  $\text{PbO}_2$ , which form when perovskites decompose. These by-products are not only hazardous but can also undergo further chemical transformation in the environment. These transformations may lead to soluble Pb salts, rendering them more mobile in water systems and ultimately deleterious to public and environmental health hazards.<sup>27</sup> Of particular concern are the inhalation of small particles of  $\text{PbO}$  during the degradation of solar cell modules, or during fire-related events, since the dispersed Pb compounds can reach deep into the respiratory system, resulting in neurological and cardiovascular abnormalities.<sup>28,29</sup> Fig. 2 presents the adsorption and distribution of Pb in the human biological system when halide perovskites degrade in the environment.

The toxic nature of Pb in PSCs underscores the importance of strict occupational safety measures during module fabrication, installation, and recycling to guarantee the safety of both workers and the communities.<sup>22</sup> The EoL management of perovskite modules is another pressing concern.<sup>31,32</sup> Without proper recycling facilities, discarded modules can be left in landfills, where the leaching of  $\text{Pb}^{2+}$  ions into groundwater becomes inevitable.<sup>33</sup> Case studies have demonstrated that populations around landfills can be exposed to Pb-containing leachates that exceed safe drinking water levels.<sup>34</sup> To quantify the risks, research has shown that simulation methods such as hail impact tests have been used to determine Pb leakage rate as expressed in eqn (2).<sup>35</sup>

$$R_{\text{Pb}} = \frac{C_{\text{Pb}} \times V}{t \times A} \quad (2)$$

where  $C$ ,  $V$ ,  $t$ , and  $A$  represent the concentration of Pb in water, volume, time, and area of the damaged PSC. Prior studies have shown that encapsulation strategies can reduce leakage rates by over 95%.<sup>36</sup> Encapsulation designs, such as multilayer polymer barriers and glass-glass lamination, have been shown to reduce Pb leakage when the module is operated at high temperatures and during accidental breakage.<sup>14</sup> The physical encapsulants have helped mitigate PSC sensitivity and enhance their



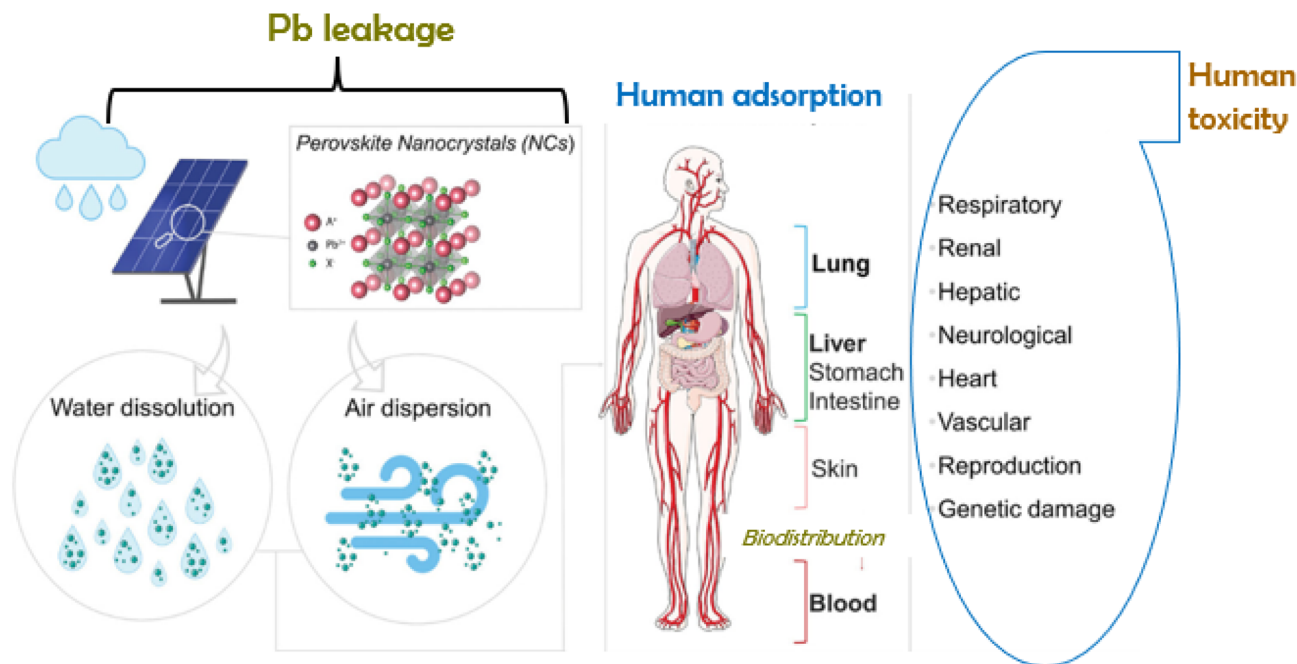


Fig. 2 Potential absorption and distribution Pb in human bodies as a result of degradation of Pb-containing perovskite that is dispersed in air and dissolved in water.<sup>30</sup>

resistance to real-world environments. Furthermore, the application of chemical additives, such as phosphate-based compounds, can stabilise Pb ions as insoluble Pb salts, thereby reducing their mobility in soil and water.<sup>15</sup> These are promising approaches; however, they must be tested under real-world conditions, including extreme weather events and long-term ageing, to ensure the module remains robust throughout its life cycle.<sup>37</sup>

#### 4. Detection of lead leakage in PSCs

Addressing Pb pollution from damaged perovskites requires sensitive detection methods and effective Pb recovery strategies.<sup>38</sup> By integrating kinetic and thermodynamic considerations, spectroelectrochemical methods such as cyclic voltammetry have been employed to understand the operational conditions of LPSCs.<sup>39</sup> Cyclic voltammetry has proven effective for probing Pb ion behaviour in monitoring and detection. This technique provides information on Pb<sup>2+</sup> adsorption, electrode kinetics, and redox processes. The reduction of Pb<sup>2+</sup> to metallic Pb, followed by oxidation to Pb<sup>2+</sup>, yields characteristic peaks that can be used for Pb quantification. Cyclic voltammetry allows for real-time monitoring of Pb leakage due to its high sensitivity to trace Pb<sup>2+</sup> quantities and the ability to distinguish complexed species from free ions.<sup>40,41</sup> A recent study by Joji *et al.*<sup>42</sup> proposed the use of biomimetic receptors immobilized on electrode surfaces to concentrate Pb<sup>2+</sup> at the electrode interface. The study suggested an effective way of improving detection limits and Pb recovery efficiency by using biomimetic ligands to immobilize Pb<sup>2+</sup>. Cycling potentials allow Pb<sup>2+</sup> to be removed from solution by reducing it at the electrode surface. Other studies have reported recovery

efficiencies exceeding 95% in Pb recovery using cyclic voltammetry, ensuring that the hazardous Pb is not only detected but also reclaimed for reuse.<sup>41,43</sup>

Remarkably, cyclic voltammetry has been used to detect Pb<sup>2+</sup> at micromolar concentrations, making it suitable for detecting Pb<sup>2+</sup> in water contaminated by decommissioned or damaged perovskite solar modules. It also ensured controlled Pb<sup>2+</sup> release by electrochemically reducing and depositing Pb on electrode surfaces. The efficacy of cyclic voltammetry for Pb detection and recovery has been enhanced by combining it with chelation strategies that bind Pb<sup>2+</sup> ions, such as gallic acid derivatives, phosphate-based polymers, ethylenediaminetetraacetic acid (EDTA)-like ligands, and crown esters. For instance, Li *et al.*<sup>44</sup> introduced dispersible gallic acid chelators into PSCs and found that they reduced Pb immobilization and leakage with improved defect passivation and perovskite grain growth. Thin polymer coatings have also been used to form highly stable complexes with Pb<sup>2+</sup>, making them suitable for *in situ* Pb immobilization.<sup>15</sup> Other studies have also shown success in “on-device Pb sequestration” by incorporating chelating agents such as ion-exchange layers and polymeric matrices.<sup>45</sup> In addition, EDTA solutions have also been used to sequester Pb ions before electrochemical reduction. Biomimetic peptides that mimic natural proteins and crown esters that provide cavity-like binding sites when incorporated in perovskite solar modules with enhanced sensitivity and selectivity in Pb detection.<sup>42</sup>

Toward this end, the use of electrochemical sensors in aqueous leachates from PSCs, water systems of soil matrices are prone to surface fouling due to deposition of degradation products, salts, or organic matter.<sup>46</sup> This deposition increases charge-transfer resistance and alters the capacitance of the



double-layered electrode, consequently leading to reduced selectivity and loss of sensitivity. The inorganic precipitates and macromolecules distort the voltametric signals by blocking the active sites. Prior reports have shown that surface fouling can be mitigated by the use of antifouling polymers, hydrophilic coatings, and nanostructured carbon coatings.<sup>47</sup> Further to this, *in situ* restoration has also been achieved by the use of catalytic surfaces or electrochemical pulsing. These antifouling strategies are known to extend sensor lifetimes. These sensors also suffer from instability of the reference electrode (typically Ag|AgCl) due to poisoning and electrode degradation.<sup>46</sup> There have been attempts to resolve this instability issue, such as the use of solid-state composite reference electrodes and sulphide-resistant Ag|AgCl electrodes. Other reports have also shown that the use of fibrous solid-state Ag|AgCl minimizes instabilities and enhance mechanical robustness of the sensor.<sup>48</sup> In addition, to quantify Pb<sup>2+</sup> in complex systems, the electrochemical sensors should have stable calibration curves. However, due to repeated recycling, the changes at the electrode surfaces and environmental fluctuations lead to calibration drift. This implies that these sensors require drift correction methods and adaptive calibration protocols.<sup>49</sup>

Prior studies on Pb quantification under regulatory or environmental conditions have underscored the importance of physical and chemical encapsulants and the dependence of leaching on test conditions. These scientific reports provide a basis for estimating the total toxic Pb that could be leached from perovskite solar modules; specific mechanisms and contributing factors to ion transport remain insufficiently understood. Various methods have been used to quantify and recover Pb from PSCs. For instance, ICP-MS has been used to give precise Pb<sup>2+</sup> concentration in aqueous leaching tests.<sup>50</sup> Additionally, closed-loop recycling with cation-exchange resins is a method employed to capture Pb from waste organic solvents, appropriate for the circular economy of PSC materials. This technique offers high binding capacity and high selectivity to Pb<sup>2+</sup>. Aqueous tests simulate practical degradation factors under moisture conditions and quantify the extent of Pb release into water systems, thereby informing relevant regulatory standards. Solvent-based methods have also been used in conjunction with aqueous methods, whereby the PSC is dissolved in a controlled medium to enable precise measurement of Pb leaching. Additionally, kinetic modelling of Pb leaching quantifies release rates under different simulated stress conditions, allowing for extrapolation of data to device lifetimes. The overall Pb recovery from various recycling and/or recovery strategies is determined using eqn (3).<sup>51</sup>

$$\eta_{\text{recovery}} = \frac{m_{\text{recovered}}}{m_{\text{initial}}} \times 100\% \quad (3)$$

In this context,  $m_{\text{recovered}}$  is the mass of Pb recovered, and  $m_{\text{initial}}$  is the initial Pb content.

Detection limits (DL) of the different detection and monitoring approaches reveal their specific analytical abilities.<sup>52</sup> DL demonstrates the lowest level of the analyte distinguishable from the background noise under optimal conditions. To ensure precision, statistical accuracy is achieved by determining

DL values multiple times. It is computed using the raw intensity data from the standard and the blank, considering eqn (4).<sup>52</sup>

$$\text{IDL} = 3\text{SD}_{\text{blk}} \times \frac{\text{STD}_{\text{conc.}}}{\text{STD}_X - \text{BLK}_X} \quad (4)$$

where IDL,  $\text{SD}_{\text{blk}}$ ,  $\text{STD}_X$ ,  $\text{BLK}_X$ , and  $\text{STD}_{\text{conc.}}$  are the instrument detection limit, standard deviation of the intensities of the multiple blank measurements, mean signal of the standard, and the concentration of the standard, respectively. Method detection limit (MDL) or IDL in comparison shows that ICP-MS has the lowest DL ( $\sim 0.001\text{--}0.01 \mu\text{g L}^{-1}$ ), demonstrating a high capability of determining the lowest level of the analyte that can be detected in the sample matrix. Conversely, encapsulation/barrier monitoring and use of chemical adsorption/scavenger layers are preventive methods that have long-term response times. They act as mitigation strategies that reduce the environmental toxicity of Pb by continually immobilizing its release from PSCs<sup>53</sup> (cf. Table 1).

The presence of Pb in the matrix of PSCs and Pb by-products resulting from material degradation currently impedes the large-scale deployment of MAPbI<sub>3</sub>-based cells.<sup>30</sup> Various techniques have been employed to quantify Pb leakage in PSCs. For instance, Pancini *et al.*<sup>50</sup> designed a fluorescent organic sensor (FS) to detect Pb leakage as MAPbI<sub>3</sub> perovskites degrade to PbI<sub>2</sub>. Pb-selective ligand binding was developed to enable measurement of the fluorescence of Pb<sup>2+</sup> ions. Simulated rainwater was exposed to the perovskite module, and sensor performance was evaluated at varying Pb<sup>2+</sup> concentrations. The researchers noted that even low levels of damage to MAPbI<sub>3</sub> solar cells could release quantifiable amounts of Pb<sup>2+</sup> into water systems. These findings suggest that damaged MAPbI<sub>3</sub> solar cells may pose severe environmental risks. Furthermore, Pancini and his co-authors introduced the potential of fluorescent organic sensors as a field-deployable technique that may be integrated into solar farm monitoring packages.<sup>50</sup>

Fluorescence signals are sensitive to humidity, ambient light, and temperature and are optimum when the signal-to-noise ratio is high.<sup>60</sup> Also, due to the presence of organic matter, interference from solar radiation, and scattering from dust, the signals can be distorted. Consequently, these sensors have been fitted with optical shielding and selective filters to minimize background interference.<sup>61</sup> Quality assurance protocols and United States Geological Survey (USGS) guidelines have also compelled researchers to ensure that the application of such systems in monitoring water systems is reliable and reproducible. Moreover, these sensors are also susceptible to reduced emission intensity and photobleaching due to prolonged UV exposure. To enhance the photostability of these sensors, the application of inorganic or organic shells has been suggested to co-encapsulate the fluorophores.<sup>62</sup> The environmental factors can also interfere with the quantitative accuracy of the fluorescence sensors. Nonetheless, the adaptive calibration schemes have been suggested to make these sensors appropriate for field applications in detecting heavy metals like Pb<sup>2+</sup> in aqueous matrices.<sup>62</sup>

Lam *et al.*<sup>63</sup> performed a multi-technique study of Pb leakage pathways in MAPbI<sub>3</sub> perovskite films. The research team





Table 1 Comparative analysis of various Pb-leakage detection and monitoring approaches in PSCs

Method	Principle of detection	Strengths	Limitations	Detection limit	Response time	Ref.
Fluorescent sensors	Enhanced Pb <sup>2+</sup> binding or fluorescent quenching	Portable, highly sensitive, and allows real-time monitoring	May suffer from interference from other ions in the matrix and requires calibration	~0.1–1 µg L <sup>-1</sup>	Seconds–minutes	54
Electrochemical sensors	Pb <sup>2+</sup> ions detected <i>via</i> changes in current/voltage at modified electrodes	It can be integrated in encapsulation layers, portable, and fast response	Unstable under long-term operation and lower sensitivity to ICP-MS	~0–10 µg L <sup>-1</sup>	Seconds	55
ICP-MS	Appropriate for environmental monitoring studies. Ionization of sample and mass ratio detection	Ultra-sensitive up to ppt levels, widely validated, and has high security	High cost, not appropriate for in-field monitoring, and requires destructive sampling	~0.001–0.01 µg L <sup>-1</sup>	Minutes–hours	52 and 56
Colorimetric assay	Visible color change upon Pb <sup>2+</sup> binding with chromogenic reagents	Low cost, does not need advanced equipment, and easy visual detection	Has limited sensitivity, semi-quantitative, and accuracy is dependent on environmental conditions	~50–100 µg L <sup>-1</sup>	Minutes	8 and 57
Encapsulation/barrier monitoring	Monitor Pb <sup>2+</sup> leakage after leakage suppression <i>via</i> engineered encapsulation	Enhances device stability, allows for self-healing, and prevents leakage rather than detecting	Requires validation for long-term performance and allows for indirect detection	Not applicable	Long-term (months–years)	58
Chemical adsorption/scavenger layers	Functional layers such as sulphides and phosphates capture Pb <sup>2+</sup>	Can be integrated in solar cell configurations and mitigates environmental contamination	Its effectiveness is dependent on material compatibility and is not a direct detection method	Not applicable	Continuous	2 and 59

utilised time-resolved photoluminescence (TRPL) to measure non-radiative recombination centres and carrier dynamics, low-dose *in situ* electron microscopy to visualise structural transformations at the nanoscale, and solid-state magic-angle spinning nuclear magnetic resonance (MAS NMR) to track ion motion and identify chemical changes in the perovskite. The research group used material simulations and modelling to validate their experimental findings. Remarkably, previous reports have shown that the electric field increases the rates of defect formation and ion migration. Vacancy formation and iodide migration have been shown to trigger the decomposition of MAPbI<sub>3</sub> into the toxic PbI<sub>2</sub>.<sup>63</sup> The acceleration of Pb<sup>2+</sup> migration, a serious ecological threat, has been reported in the presence of electric fields. The authors have also identified the importance of crystalline and morphology as crucial to the durability of the device. Their work also highlighted the complex interrelationship between material stability and electric fields in defect accumulations and ion migration.

Another promising approach to monitoring Pb leakage is the use of electrochemical sensors.<sup>64</sup> They are selective electrode-based Pb<sup>2+</sup> sensors that detect changes in ionic concentration in water. Recent findings have confirmed that electrochemical detection is sensitive and has high response times, making it a suitable technique for tracking the degradation of perovskite modules in real-time under outdoor conditions.<sup>65</sup> Unlike fluorescence-based methods, electrochemical sensors can be integrated into low-cost monitoring systems, providing a scalable approach to large solar farms.<sup>66</sup> In addition to laboratory detection, field-deployable kits are being developed to monitor the presence of Pb on the ground. Portable colorimetric assays entail chromogenic reagents that change colour when Pb<sup>2+</sup> ions are present.<sup>67</sup> These kits allow non-experts to quickly determine the contamination levels in soil and water surrounding perovskite installations. These are inexpensive and less sensitive than ICP-MS or TRPL, but they can be used in preliminary screening and community-wide surveillance, especially in areas with limited well-developed laboratory infrastructure.

ICP-MS is an indispensable technique when ultra-trace level and high-accuracy quantification is required. It can measure Pb<sup>2+</sup> levels to parts-*per*-trillion (ppt) and parts-*per*-million (ppm) with exceptional precision.<sup>68</sup> This method allows assessments of environmental risks and compliance with strict standards, including the US Environmental Protection Agency (EPA) and the EU Regulation on Registration, Evaluation, Authorization, and Restriction of Chemicals (REACH), where electrochemical or colorimetric techniques lack sensitivity.<sup>59</sup> It is also robust for handling complex systems, particularly when Pb<sup>2+</sup> leaches into biological, water, or soil samples with minimal interference. ICP-MS has been applied to quantify Pb<sup>2+</sup> leakage with high precision over time, to examine degradation pathways of MAPbI<sub>3</sub>-based PSCs, and to correlate Pb mobilization with degradation factors, encapsulation strategies, and PSCs architectures.<sup>17</sup> Also, it provides isotopic resolution, allowing differentiation between Pb<sup>2+</sup> from damaged or degraded PSCs and background contamination for regulatory reporting and gaining mechanistic insights. It is well-established that complex matrices distort signals and induce interference in simple

assays; thus, ICP-MS with mass filtering and plasma ionization is required to meet strict standards and conduct environmental risk assessments.<sup>50,69</sup> Simple techniques may not be suitable because internationally accepted accuracy is needed in litigation and certification. Thus, the advanced monitoring of complex environmental contaminants and toxic metals, including Pb, cannot be conducted without high-resolution analytical techniques, including ICP-MS.<sup>69</sup> The detection limit of Pb in water can be modelled using eqn (5).<sup>70</sup>

$$L_{\text{detection}} = k \times \frac{\sigma_{\text{blank}}}{S} \quad (5)$$

Here,  $k$ ,  $\sigma_{\text{blank}}$ , and  $S$  are a constant, the standard deviation of the blank measurements, and sensitivity, respectively.

In Pb quantification, however, simple methods and low-cost detection, such as portable electrochemical probes, colorimetric analysis, and fluorescent sensors, are employed in routine screening and monitoring.<sup>71</sup> Remarkably, these techniques can be adequate in quality control in device fabrication and preliminary screening. Moreover, these simple, portable, and inexpensive methods also work well in on-site testing and community-level monitoring. For instance, fluorescent sensors have been utilized to monitor  $\text{Pb}^{2+}$  leaching without requiring complex instrumentation.<sup>72</sup> This democratization of  $\text{Pb}^{2+}$  detection is consistent with the JT to clean energy, ensuring that PSCs can be fabricated and the leaching of the hazardous Pb can be monitored even in resource-limited settings without prohibitive costs.<sup>73</sup> Accordingly, simple methods used in  $\text{Pb}^{2+}$  detection serve as complementary techniques rather than exclusive, since they provide benchmark precision and broad monitoring capability. Simple techniques such as electrochemical sensors are field deployable and affordable, thus significant in the detection of emerging pollutants within water systems.<sup>73,74</sup>

Advanced spectroscopic methods have also been used to investigate Pb leakage pathways. X-ray photoelectron spectroscopy (XPS) and X-ray absorption near-edge structure (XANES) have been employed to determine the chemical state of Pb in degraded perovskite films.<sup>75</sup> These methods provide insight into the oxidation and conversion of  $\text{PbI}_2$  to other Pb oxides or salts, which dictate mobility and toxicity. Such approaches are not field-deployable but are necessary to understand the fundamental chemistry of degradation and to develop more resilient perovskite formulations. Recent ICP-MS and accelerated ageing experiments have shown that multilayer polymer encapsulants and glass-glass encapsulation can significantly reduce  $\text{Pb}^{2+}$  release under simulated rainfall and humidity.<sup>76</sup> However, as encapsulation layers are degraded by mechanical stress or weathering, the leakage increases exponentially. This highlights the importance of combining detection methods with durability tests to predict long-term risks. Combined monitoring systems that connect multiple detection methods to form a cumulative risk evaluation are also critical in analysing perovskite degradation. Fluorescence sensors, for example, may be combined with ICP-MS validation and electrochemical probes to provide high-precision laboratory validation and rapid field measurements.<sup>50</sup> Such hybrid solutions can ensure

that both short-term and long-term monitoring needs are met, allowing regulatory authorities and industry leaders to implement safety standards in the scale-up of PSCs. These frameworks represent a significant step toward achieving a balance between the extreme efficiency of perovskites and the need to ensure environmental safety.

The  $\text{Pb}^{2+}$  monitoring and detection applications are constrained by several factors. Since PSC modules are expected to reduce costs per watt due to scaling,  $\text{Pb}^{2+}$  leaching monitoring infrastructure continues to be a hidden cost. For instance, ICP-MS is an expensive instrument that demands skilled operators to calibrate the instrument and analyse the spectra.<sup>72</sup> Colorimetric, electrochemical, and fluorescent methods have the advantage of being portable, but their accuracy under real-world conditions (UV-radiation, dust, and humidity) remains uncertain.<sup>77</sup> In addition, scavenger/encapsulation layers to immobilize Pb need precise deposition, increasing the costs for scale fabrication of PSCs. Generally, the degradation pathways tend to be non-linear and often environmentally dependent, making the release of  $\text{PbI}_2$  and  $\text{Pb}^{2+}$  difficult to detect, thus compromising the efficacy of Pb detection and monitoring techniques.<sup>78</sup> Finally, the implementation of these monitoring methods faces impediments related to strict policy frameworks, which may delay the commercialization and certification of laboratory breakthroughs.

## 5. Mechanisms of $\text{MAPbI}_3$ decomposition and lead leakage

PSCs are semiconductor materials that have chemical components that exhibit weak bonding through ionic interactions, hydrogen bonding, and van der Waals forces. PSCs containing Pb can be hazardous to the environment and public health since degradation ions such as  $\text{Pb}^{2+}$  can readily migrate to various layers when exposed to degradation environments (Fig. 3). Unlike the widely deployed silicon solar cells, perovskites designed for outdoor applications are susceptible to damage due to natural factors such as wind stress, snow, hailstorms, or fires during operation.<sup>18</sup> Improved understanding of possible health and environmental hazards and strategies for management will make LPSCs commercially viable and sustainable. The degradation mechanisms of perovskites are associated with intrinsic and extrinsic factors arising from the crystallographic or the molecular structure of the perovskite and inherent practical application conditions.

### 5.1. Intrinsic degradation factors

Previous studies have discussed hysteresis, crystal defects, ion migration, optical absorption limitation, and thermal instability as common factors that impede the intrinsic stability of perovskites.<sup>80,81</sup> The open circuit voltage ( $V_{\text{oc}}$ ) of perovskites is correlated with electron and hole separation quasi-Fermi levels within the perovskite layer during illumination.<sup>82</sup> Therefore, the presence of defect-induced non-radiative recombination processes reduces the quasi-Fermi level splitting, thereby lowering the  $V_{\text{oc}}$ .<sup>81</sup> Besides, fill factor (FF) is also dependent on



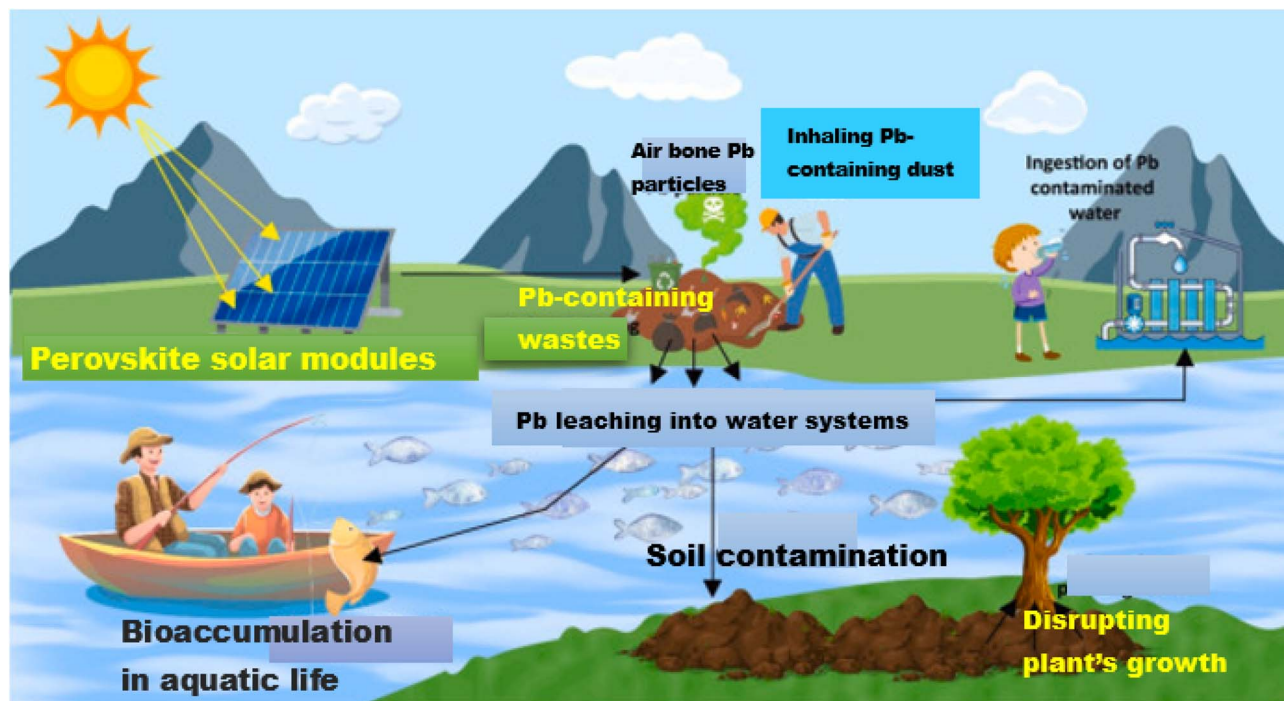


Fig. 3 Overview of Pb leakage in the environment from perovskite solar modules.<sup>79</sup>

the  $V_{oc}$ , and thus, these defects that arise from antistites substitutions, interstitials, and atomic vacancies also decrease the FF. The loss of volatile  $\text{MAPbI}_3$  results in the creation of iodide vacancies and, consequently, trap states in the device.<sup>81</sup> During degradation,  $\text{Pb}^0$  also forms, increasing non-radiative recombination and inhibiting efficient charge transfer. In addition, the presence of defect density at the grain boundary also affects perovskite performance by lowering  $V_{oc}$  and  $J_{sc}$ . The presence of Frenkel defects also contributes to hysteresis due to repetitive charging and discharging cycles.<sup>83</sup> Under thermal drift or bias voltage, the cations and anions in the perovskite migrate within the perovskite, causing device instability. Ion migration has been reported to alter the crystal structure and relocate traps, leading to lattice collapse in perovskites and ultimately influencing device performance. The migration ions may also move to other functional layers of the perovskite, including the electron transport layer (ETL), hole transport layer (HTL), and electrodes, potentially corroding these layers, as shown in Fig. 4. The corrosion of these functional layers significantly reduces interlayer conductivity and forms a stable silver iodide ( $\text{AgI}$ ) compound that is detrimental to the device's overall performance.<sup>81</sup>

Previous studies have shown that hysteresis due to defect accumulation at the transport layer/perovskite interface reduces device stability. While the origin of these defects is still under serious investigation, it is crucial to estimate their concentration and location using impedance spectroscopy. Typically, impedance spectra show a high-frequency response associated with dipole depolarisation, ionic diffusion, chemical capacitance, or geometric capacitance within the active layer.<sup>80</sup> It also gives the low-frequency responses associated with factors such

as ionic diffusion, device degradation, trap states, electron accumulation at interfaces, and dielectric effects.<sup>80</sup> Notably, impedance spectra reveal the origins of ion defects, but conflicting interpretations hinder improved understanding of device hysteresis.

## 5.2. Extrinsic degradation factors

During solar cell operation, halide PSCs interact with external factors, including electric bias, oxygen, moisture, light, heat, or external agents. Light induces the redistribution of metal and halide ions in the  $\text{MAPbI}_3$  film. This results in increased photoluminescence due to iodide migration. Light-induced ion migration causes film segregation, resulting in halide-deficient and halide-rich regions.<sup>84</sup> The interaction of oxygen with the perovskite layer results in the formation of highly reactive superoxide species, generated by the photolysis of water. This light-induced degradation induces vacancy migration in the perovskite film, leading to a decline in device performance. In addition, perovskites are known to be stable within particular temperature ranges. Under heat,  $\text{MAPbI}_3$  may decompose into methyl iodide, ammonia, and lead iodide ( $\text{PbI}_2$ ) at temperatures exceeding  $85^\circ\text{C}$  in an inert atmosphere.<sup>84</sup> Perovskites predominantly use organic ETLs and HTLs, which can degrade at elevated temperatures. When HTLs are exposed to oxygen, the hole-transport barrier increases, reducing hole extraction at the HTL/perovskite interface. Moreover, the perovskite reacts with oxygen in the presence of water, which is an irreversible chemical process. Light-induced degradation has been mitigated through advanced device encapsulation strategies. A good encapsulant ensures Pb immobilization by capturing ions if the



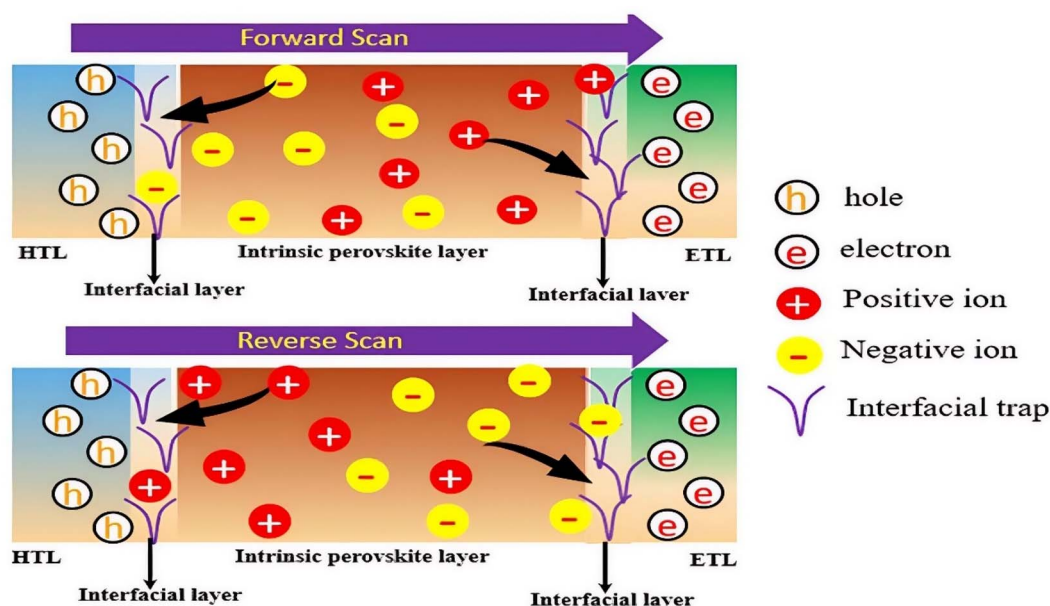


Fig. 4 Ion migration and re-orientation in the perovskite under forward and reverse scans.<sup>80</sup>

device is broken or damaged.<sup>85</sup> Table 2 summarises studies that have been conducted to enhance device stability and ensure Pb immobilization, with promising results. Formamidinium iodide (FAPbI<sub>3</sub>) and MAPbI<sub>3</sub> are highly hygroscopic and readily decompose into their respective precursor ions.<sup>86</sup> Therefore, when exposed to humidity, water molecules form weak hydrogen bonds with organic molecules within the device structure. Without physical encapsulants, perovskite films cannot withstand continuous exposure to humidity and fail the damp-heat test, which involves 85% relative humidity.<sup>85</sup> Accordingly, both extrinsic (environmental) and intrinsic

(chemical) factors need to be considered before the deployment and commercialization of PSCs.<sup>81</sup>

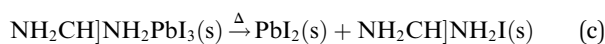
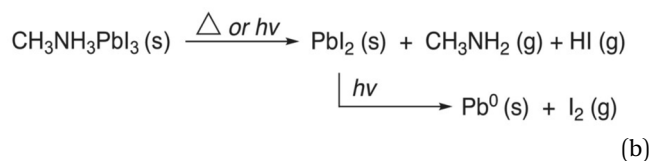
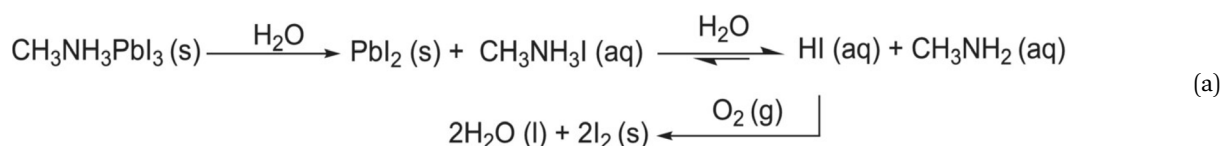
Pb-related environmental and public health impacts are measured as a function of exposure risk. Exposure probability depends on mobility, concentration, and the presence of toxic constituents in the environment. MAPbI<sub>3</sub> is known to undergo various degradation pathways and seep into soil and water systems, circulating in the atmosphere and natural ecosystems. Under humid environments, MAPbI<sub>3</sub> (CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>) decomposes into CH<sub>3</sub>NH<sub>3</sub>I and PbI<sub>2</sub> according to Rxn (a). Subsequently, CH<sub>3</sub>NH<sub>3</sub>I undergoes deprotonation by water

Table 2 Proposed encapsulants of PSCs with reported device performance and test conditions

Encapsulation material	Initial PCE	Durability of the standard test	Conditions	Retention of peak PCE	Standardized tests performed	Ref.
Thiol-functionalized perfluoroalkyl	21.79%	500 h	85 °C, MPP at N <sup>2</sup> -filled chamber	90.1%	No	87
Polyacrylic acid (PAA) ionogel	22.87%	1000 h	Room temperature 85% RH	95%	Damp heat, thermal cycling	88
		200 cycles	–40 to 80 °C cycling	96.1%		
DMDP (front), EDTMP-PEO (back)	20.27%	500 h	MPP at room temperature	80%	No	45,89
Multilayer Al <sub>2</sub> O <sub>3</sub> and pV3D3	20.1%	300 h	50 °C, 50% relative humidity, dark	98.9%	No	90
Alucone and Al <sub>2</sub> O <sub>3</sub> bilayer stack	17.01%	2100 h	30 °C, 80% relative humidity, dark	96%	No	91
Al <sub>2</sub> O <sub>3</sub> and 1H, 1H, 2H, 2H-perfluoro decyl-trichlorosilane stack	19.7%	500 h	85 °C, 85% relative humidity	78%	Damp heat not long enough	
PIB wide blanket	19%	1800 h	85 °C, 85% relative humidity	95%	Damp heat and humidity freeze	92
		30 cycles	–40 to 80 °C cycling	95%		
Resin UVR-C (front), C100 (back)	25.5%	500 h	Ambient conditions	97%	No	93
Sulfonic acid-based resin	20.1%	500 h	45 °C, MPP, ambient RH	83%	No	94



molecules, producing  $\text{CH}_3\text{NH}_2$  and HI. Further, HI decomposes into water and  $\text{I}_2$  in the presence of oxygen. Under elevated temperature,  $\text{MAPbI}_3$  degrades to produce  $\text{PbI}_2$  and  $\text{CH}_3\text{NH}_3\text{I}$ , which then decomposes into HI gas and  $\text{CH}_3\text{NH}_2$ , as shown in Rxn (b). Similarly,  $\text{FAPbI}_3$ -based perovskite degrades when exposed to temperatures above  $230^\circ\text{C}$ , as depicted in Rxn (c). Boyen *et al.*<sup>95</sup> conducted a simulated fire experiment showing that burning PSCs release  $\text{PbI}_2$  into the smoke. These findings suggested that Pb compounds disperse in the air, polluting the environment.<sup>18</sup> Therefore, the degradation factors of perovskite materials induced by heat and, to a greater extent, ultraviolet radiation cannot be underestimated. It is well-established that ultraviolet radiation degrades organic cations in the perovskite material, leading to chemical decomposition and phase segregation, as shown in Rxn. (b).



Under degradation considerations,  $\text{MAPbI}_3$  decomposes to form  $\text{PbI}_2$ , a significant environmental concern.  $\text{PbI}_2$  is insoluble in water, with a solubility constant ( $K_{\text{sp}}$ ) of  $8.0 \times 10^{-9}$  to  $1.84 \times 10^{-8}$ .<sup>96</sup> This compound cannot be dissolved in water; however,  $\text{PbO}$  powder can be absorbed through human skin, posing serious health risks. Severe Pb exposures can be classified as accidental, disposal-related, or due to harsh weather conditions. The processing of perovskites may involve toxic solvents that can Pb to accidents by inhalation, ingestion, and even contact with the skin.<sup>97</sup> Further, there are risks associated with module-induced breakage of Pb due to the density of the material and combustion during waste disposal of Pb-based solar modules.<sup>34</sup> Other potential sources of Pb exposure related to perovskite solar technologies include severe weather events (such as hurricanes, tornadoes, and hailstones) and transport-related risks (such as vehicle collisions). Risk exposure pathways, including landfill leaching and groundwater and soil contamination, should be well understood to mitigate Pb leakage. Although the efficiencies are impressive,  $\text{MAPbI}_3$  formulations have been found to degrade in the presence of

water, heat, and light, releasing Pb-based by-products such as lead carbonate, lead phosphate, lead iodide, and lead hydroxide.<sup>18</sup> The routes of exposure and the risks that  $\text{MAPbI}_3$  may pose are multi-pathways, varying in risk levels based on pre-existing contamination levels, concentration, and source,<sup>98</sup> as summarised in Table 3.

## 6. Recent advances in the prevention of lead leakage in LPSCs

Physical encapsulation (Fig. 5) is the most widely used method to ensure that PSCs remain Pb-leakage-free.<sup>18,99</sup> Encapsulation refers to the use of protective layers, such as glass-glass lamination, polymer films, or multilayer composites, that block water, oxygen, and mechanical forces.<sup>18</sup> Glass-glass

encapsulation, in particular, has been shown to reduce  $\text{Pb}^{2+}$  leakage by more than 90% under simulated rainfall conditions, and this effectiveness is also observed in the real world.<sup>100</sup> Recent advancements use internal encapsulation, which involves using materials that interact with Pb to prevent its migration or capture it. In contrast, external encapsulants serve as physical barriers to prevent degradation due to harsh conditions and minimise Pb leakage. Fig. 5 depicts the external and internal encapsulation of PSCs. Nevertheless, encapsulation is not without challenges: microcracks, delamination, and thermal expansion mismatches can degrade barrier integrity over time, especially under harsh weather conditions. Thus, while encapsulation provides a physical barrier, its ultimate success depends on structural design and material reliability.<sup>76</sup> Chemical absorption strategies complement physical barriers, actively immobilising  $\text{Pb}^{2+}$  upon release from degraded perovskite films.<sup>15</sup>  $\text{Pb}^{2+}$  also interacts with absorbent compounds (phosphates, sulfates, and carbonates) to form insoluble salts such as  $\text{Pb}_3(\text{PO}_4)_2$  or  $\text{PbSO}_4$ , which are more stable and less mobile in the environment. An example is the use of phosphate-based additives incorporated into encapsulation layers, which are reported to reduce Pb leakage by up to 96% compared to unencapsulated devices.<sup>58</sup> Functionalized polymers and nanomaterials that incorporate chelating functional groups (*e.g.*, thiols, amines) have also been designed to selectively trap  $\text{Pb}^{2+}$ , thereby capturing them within the device infrastructure. The techniques not only reduce environmental risks but also enhance device stability by reducing ion migration routes.<sup>101</sup>

Hybrid designs that utilise the integrated strength of physical encapsulation and chemical absorption are gaining popularity as efficient methods for preventing leakage.<sup>18</sup> By



Table 3 Potential lead exposure pathways using lead-based modules

Value chain stage	Causation	Health and safety risk type
PSC design	Identification of Pb vs. non-Pb containing perovskites	N/A
Device fabrication	Manufacturing process	Contaminated effluence
	Solvent selection	Skin contact
	Machining process	Inhalation
Transportation and staging	Improper transportation or packaging	Skin contact
	Accident during transportation	
Installation	Breakage/damage during installation	Skin contact
Operation	Aging	Water and soil system contamination
	Weather	Skin contact
	Fire	Inhalation
End-of-life management	Landfill or recycling process	Water and soil system contamination
	Disassembly, staging, and transportation	Skin contact Inhalation

incorporating Pb-absorbing agents to encapsulation layers, researchers have developed dual-protection systems that should not only prevent external stressors but also repair any Pb ions that escape.<sup>15</sup> For instance, the encapsulation of phosphate-based scavengers into polymer encapsulants has been more effective in hail, fire, and heavy rain environments and has released significantly less Pb than when encapsulated.<sup>58</sup> Moreover, self-healing encapsulation materials provide an additional layer of resilience. These polymers can self-heal microcracks caused by mechanical stress, thereby preserving both the physical barrier and chemical scavenging properties over extended working lifetimes.<sup>102</sup> These hybrid systems represent a promising avenue for realising commercial-scale deployment of perovskites. Even though encapsulation and absorption strategies are effective when functioning, Pb leakage cannot be avoided unless a lifecycle view is applied that covers fabrication, usage, and EoL handling.<sup>103</sup> Recycling protocols that integrate encapsulation removal and Pb recovery are crucial in preventing landfill contamination. Closed-loop recycling, which involves recycling recovered Pb and incorporating it into new perovskite devices, not only reduces environmental risks but also makes PSC technology consistent with the principles of a circular economy.<sup>76</sup> Life cycle analysis studies have shown that recycling and recovery can reduce the toxicity footprint of perovskites compared to silicon photovoltaics.<sup>104</sup> Thus, leakage prevention

must be incorporated throughout the entire value chain, including material design and disposal, to ensure that PSCs are not only high-performing but also environmentally sustainable.

### 6.1. Sustainable decommissioning of perovskite modules

Although perovskite commercialisation is still in its infancy, the issue of recycling has been widely debated in the context of sustainable technologies.<sup>105</sup> Successful EoL management of LPSCs relies on an enhanced understanding of the device life cycle, which is crucial (Fig. 6).<sup>106</sup> The first step in decommissioning LPSCs is to identify its critical components. This intricate journey begins with sourcing raw materials, including the absorber layer, and sustainable fabrication for creating small-area perovskites to minimise efficiency losses.<sup>106</sup> The material components can be categorised by their cost and sustainability, and the urgency for recycling can be determined accordingly.

Directive 2008/98/EC (Fig. 7(a)) outlines the waste hierarchy pyramid, which can be used to inform the sustainable decommissioning of PSC modules.<sup>105</sup> At the top is prevention, which involves embedding eco-design principles into solar cell design, such as the use of physical encapsulants and the incorporation of durable and stable materials. In addition, perovskite modules contain valuable materials, including transparent conductive oxides, halides, Pb, and tin, which can be reused or

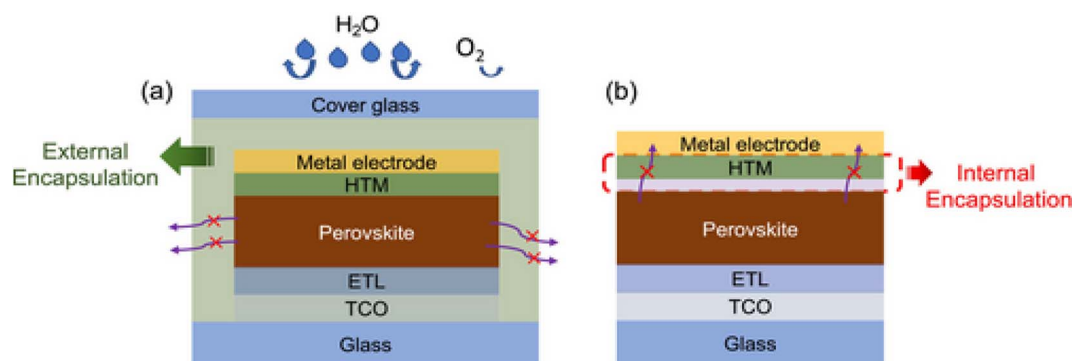


Fig. 5 Physical encapsulation of perovskites to capture and prevent lead migration: (a) external encapsulation and (b) internal encapsulation.<sup>18</sup>



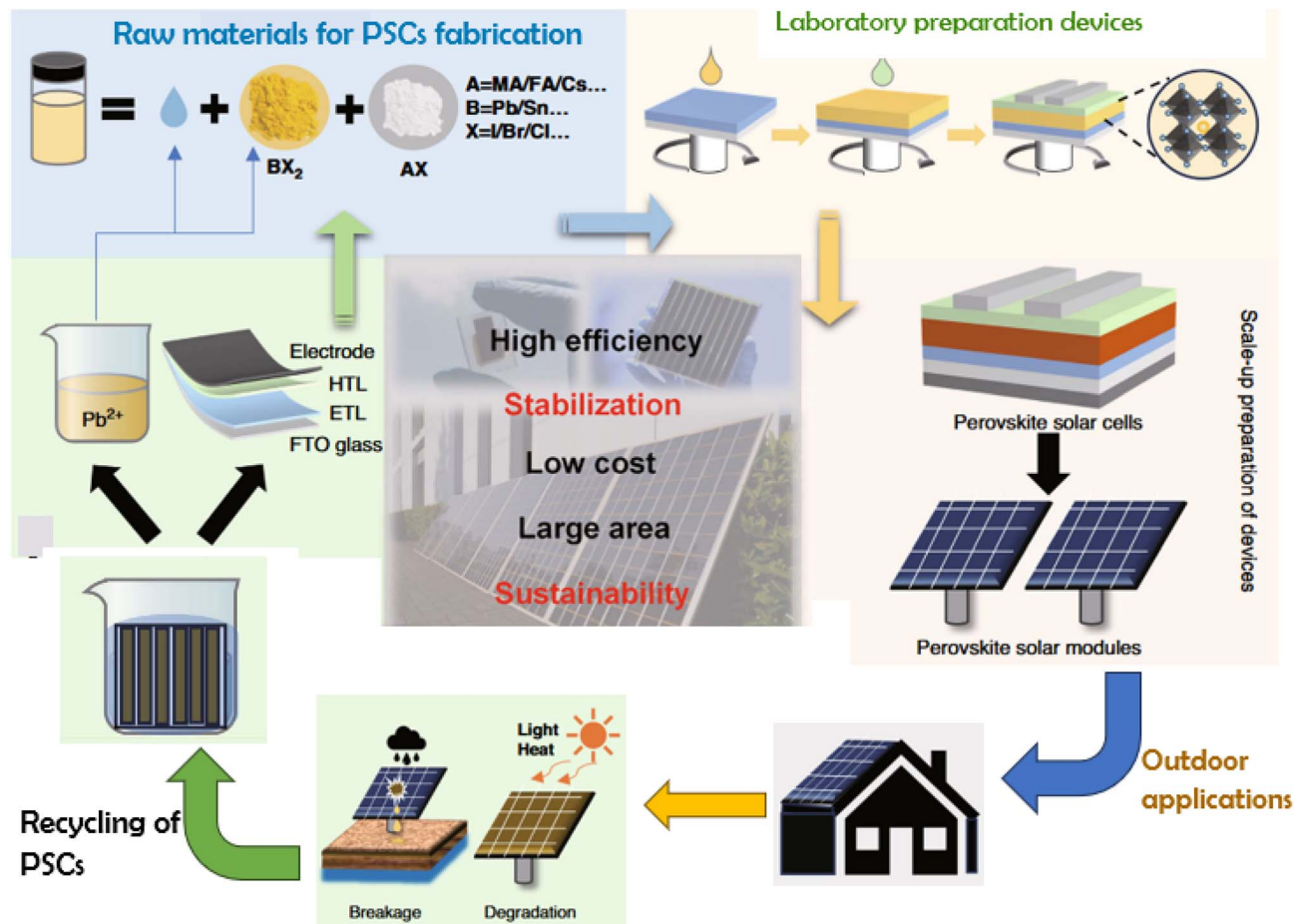


Fig. 6 Lifecycle of perovskite solar technology.<sup>106</sup>

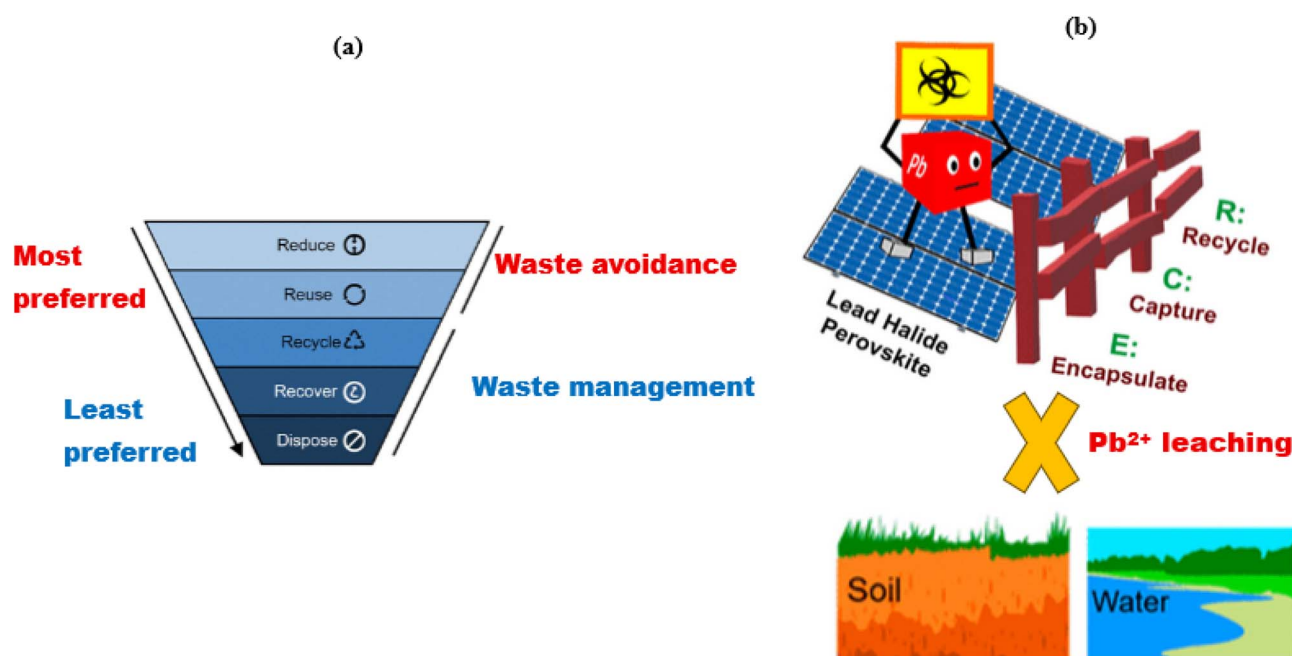


Fig. 7 Waste hierarchy pyramid as outlined in the directive 2008/98/EC of the European Parliament and of the Council of 19 November 2008 on wastes and repealing certain directives<sup>105</sup> (a) and (b) emerging approaches for waste management of perovskite solar modules.<sup>103</sup>



recycled *via in situ* regeneration, solvent extraction, and chemical precipitation. Notably, recycling these materials supports the circular economy and simultaneously prevents the leaching of toxic contaminants from hazardous waste into the environment. In the lower tiers of the hierarchy, (energy recovery and disposal), requires that wastes can be incinerated or disposed of on land fields, but should remain as the last pathway for waste management.<sup>105</sup> Encapsulate, capture, and recycle (ECR) are emerging material chemistry approaches that have been investigated to potentially mitigate the health and environmental hazards associated with LPSC devices,<sup>51</sup> as illustrated in Fig. 7(b).

*In situ* recycling of the perovskite layer is an emerging technique that mitigates Pb leakage, a common issue during perovskite recycling. Unlike the energy-intensive recycling strategies such as chemical precipitation, thermal treatment, and solvent extraction, *in situ* recycling minimizes these processing steps and directly regenerates  $\text{PbI}_2$ . Xu *et al.*<sup>107</sup> demonstrated that  $\text{PbI}_2$  can be recovered and reintroduced into devices, resulting in robust performance comparable to that of devices fabricated with fresh precursors. Remarkably, differences in environmental benefits, including *in situ* recycling, support the circular economy in perovskite device fabrication, thereby reducing overall material costs. This paradigm shift aligns with the European Union directive 2008/98/EC on waste management, which prioritises recycling, reuse, and prevention.<sup>108</sup>

## 6.2. Recovery of material components from LPSCs

Few studies have been conducted beyond the recovery and reuse of perovskite material components, specifically focusing on  $\text{Pb}^{2+}$ .<sup>109</sup> The sustainability and feasibility of recycling perovskite modules are crucial in the design of future perovskite devices. Common LPSC materials, along with their advantages, disadvantages, and recycling implications, are summarised in Table 4. Transparent conductive oxide (TCO) substrates and gold contacts are the most environmentally impactful and expensive materials used in halide perovskites. Research has shown that gold can contribute up to 65% of the carbon footprint and constitute up to 90% of the embedded material cost, due to the energy requirements during its deposition and the material value.<sup>110</sup> The process of recovering perovskites enables the reuse of the recovered foil, but this remains a scientific challenge. Before reuse, these foils should be melted into suitable gold wires/pellets, which is an energy-intensive process, and may not be economically viable for large-scale commercialisation.<sup>110</sup> However, due to its material benefits, such as high conductivity and stability, gold remains preferred in device configurations that support circular economy.

Before recovering the device components, the perovskite to be recycled is first peeled off to expose the film. The perovskite is then dissolved in organic solvents such as DMF, dimethyl sulfoxide (DMSO), and nontoxic butylamine (BA).<sup>111</sup> Previous reports on the use of polar solvents yielded a solution containing  $\text{Pb}^{2+}$ , followed by separation and extraction of  $\text{PbI}_2$  using precipitants or adsorbents for reuse in new devices.<sup>112</sup>

DMF has been successfully used as a solvent to dissolve EoL perovskites to obtain  $\text{Pb}^{2+}$ , followed by the addition of Fe-decorated hydroxyapatite hollow composite with a negative surface charge to adsorb  $\text{Pb}^{2+}$ . Subsequently, water can be added to the resulting solution to dissolve it, and KI is then added to obtain pure  $\text{PbI}_2$ . This method has been successfully used to obtain a recycling yield of 99.97%.<sup>112</sup> Similarly,  $\text{Pb}^{2+}$  can be adsorbed by the cation exchange resin (CER) method with a remarkable recycling rate of 99.99%.<sup>51</sup>  $\text{PbI}_2$  is then separated and extracted by reacting with the solution containing NaI and  $\text{HNO}_3$ , as shown in Fig. 8(a). Other studies have also suggested using the eutectic solvent ethylene glycol and choline chloride to dissolve the perovskite and separate  $\text{Pb}^{2+}$  from the solvent by electrodeposition, achieving a Pb recycling rate of 99.8%.<sup>102</sup> In addition,  $\text{NH}_3 \cdot \text{H}_2\text{O}$  can also be used to achieve similar extraction results.<sup>113</sup> Fundamental studies have also explored *in situ* recycling of  $\text{MAPbI}_3$  by dissolving the HTL in chlorobenzene and using a tape to strip the Ag electrode.<sup>107</sup> Subsequently,  $\text{PbI}_2$  is then obtained by the thermal degradation of  $\text{MAPbI}_3$ . Afterwards, a re-spin coating of MAI is performed on the  $\text{PbI}_2$  layer to form a new perovskite film (Fig. 8(b)). The performance of the re-prepared devices (14.84%) was higher than that of the control devices (14.35%).<sup>107</sup> Performances of re-prepared devices can be better enhanced by the use of hydroxypropyl- $\beta$ -cyclodextrin crosslinked with 1,2,3,4-Butanetetracarboxylic acid (HP $\beta$ CD-BTCA), which can chelate  $\text{Pb}^{2+}$  as a  $\text{Pb}^{2+}$  adsorbent and as a passivator of the perovskite.<sup>114</sup> The resulting composite of HP $\beta$ CD-BTCA@ $\text{PbI}_2$  can be used, and the PCE of the as-prepared devices reached 20% higher than that of the control devices (19.63%).<sup>114</sup> Besides, the  $\text{PbI}_2$  recovered from HP $\beta$ CD-BTCA@ $\text{PbI}_2$  composite material showed a purity of 98.9%.<sup>114</sup>

Ion migration may also lead to the degradation of PSC materials, resulting in irreversible changes to the material properties of HTL.<sup>110</sup> Furthermore, the use of encapsulants such as ethylene-vinyl acetate (EVA) complicates the recycling process due to their chemical stability and strong adhesion. Innovative approaches introduced to overcome this challenge include the use of New Industrial Encapsulation (NICE).<sup>79</sup> Moreover, the use of elastomers and thermoplastics has been proposed as an alternative to offer superior delamination properties compared to EVA.<sup>116–118</sup> The EoL recycling of perovskite modules may also be hindered by the use of highly toxic antisolvents, such as chlorobenzene and toluene, as well as by solvents such as dimethylformamide. The perovskite precursors are also required for the selective recovery of materials from weathered or damaged perovskites, posing significant health and environmental risks. This underscores the need for sustainable and eco-friendly fabrication techniques, such as the use of green solvents (*e.g.*, water, ethanol, and methanol) and green antisolvents (*e.g.*, 2-methyltetrahydrofuran and anisole). Apart from the use of green solvents and antisolvents, it is also necessary to design HTLs that are highly soluble in green solvents.<sup>118</sup>

Recycling can be challenging due to conflicts or overlaps of the material's thermal and chemical properties. Previous studies proposed integrating AI algorithms to develop a more comprehensive understanding of the optimal recycling strategy,



Table 4 Material layers used in PSCs with advantages, limitations, and recycling implications<sup>79</sup>

Material layer	Material options	Advantages	Limitations	Recycling implications
Substrate	Glass	Excellent thermal stability Strong barrier against moisture and chemicals	Rigid Relatively expensive	Highly compatible with mechanical recycling Can be integrated into existing silicon PV recycling streams
	Polymers (PET, PEN)	Flexible and lightweight Lower cost	Poor heat resistance Brittle under stress	Recycling is challenging under harsh thermal/chemical treatments
Transparent conducting electrode	FTO (fluorine-doped tin oxide)	Good thermal stability Cost-effective	Higher surface roughness	Durable and less prone to degradation during recycling
	ITO (indium-doped tin oxide)	Smooth surface High optical transparency	Lower thermal stability Expensive	Recycling is critical to recover indium, a scarce raw material
ETL (electron transport layer)	Inorganic (TiO <sub>2</sub> , SnO <sub>2</sub> , ZnO)	Stable Low-cost Easy fabrication	Strong adhesion to substrates complicates separation	Difficult to recycle due to tight bonding with substrates
	Organic (PCBM)	Low processing temperature	Poor stability Low electron mobility	Degrades under heat/solvent exposure Removal requires toxic solvents (e.g., chlorobenzene)
				Strong adhesion reduces recyclability
HTL (hole transport layer)	Inorganic (NiO <sub>x</sub> , CuSCN)	Chemically and thermally stable Cost-effective	Possible interfacial reactions	
	Organic (PEDOT:PSS, spiro-OMeTAD, PTAA)	Solution-processable Enhanced charge transport	High cost Complex synthesis, poor long-term stability	Dopants complicate chemical separation during recycling
Perovskite layer	Pb-based	High efficiency	Toxicity concerns	Pb recovery is essential to prevent environmental contamination
	Tin-based	Non-toxic	Easily oxidized Air instability	Oxidation complicates recovery and reuse
	Bismuth-based	Stable Low toxicity	Low efficiency Early-stage technology	Recycling pathways are not yet established
Back electrode	Gold (Au)	Excellent conductivity High work function	Very expensive. Requires vacuum deposition	Can be selectively etched and recovered
	Silver (Ag)	Lower cost than gold	Diffusion into perovskite Requires vacuum deposition	Recoverable, but diffusion complicates separation
	Copper (Cu)	Low cost Good conductivity	Prone to oxidation	Residual halides contaminate copper during recycling
	Carbon (C)	Cheap Chemically inert	Low work function	Difficult to isolate during recycling

which could help recover the most valuable, costly, or hazardous materials.<sup>119</sup> During recycling, it is also scientifically feasible to recover highly pure materials that deliver efficiencies comparable to those of pristine photovoltaics. Recycling involves mechanical, thermal, or chemical treatment of materials, which can increase the propensity for material contamination or damage, potentially introducing unintentional dopants that affect material performance.<sup>14</sup> Therefore, recycling strategies may not be relied upon due to reproducibility issues and inconsistent performance. Furthermore, thermal and solvent-based recycling methods pose environmental challenges. Pb-containing compounds may volatilize into the environment, posing significant risks of Pb contamination.<sup>109</sup> Aprotic solvents such as DMF may lead to the generation of toxic solvent waste, increasing health and environmental risks.<sup>79</sup> PSCs are fabricated from nanoscale materials, and the recovered materials from recycling are often minimal; the cost of layer-by-layer purification may outweigh the device's market value.<sup>120</sup> Recycling is also a high-energy-intensive process,

particularly during the thermal recovery processes.<sup>121</sup> According to previous studies, the LCA of recovering valuable materials from waste perovskites, such as aluminium, glass, Pb, nickel, gold, and silver, indicates that the total cost calculated for recovery ranges from the most effective method to the least (\$10.70–\$32.45).<sup>122</sup> A summary of challenges in Pb recycling is presented in Fig. 9.

### 6.3. Closed-loop recycling of lead

Although Pb remains a hazardous element, innovative approaches are being developed to mitigate the toxicity of LPSCs. Researchers are also addressing recycling and recovery methodologies to mitigate the environmental risks associated with Pb leaks to enable the re-use of useful materials. For instance, *in situ* regeneration in real-time has been proposed to restore Pb directly within the device, rather than precipitating or dissolving the device. Real-time monitoring implies tracking the changes in MAPbI<sub>3</sub>-PSCs “as they happen,” generally with second-to-minute resolution. Unlike in *ex situ* monitoring, the



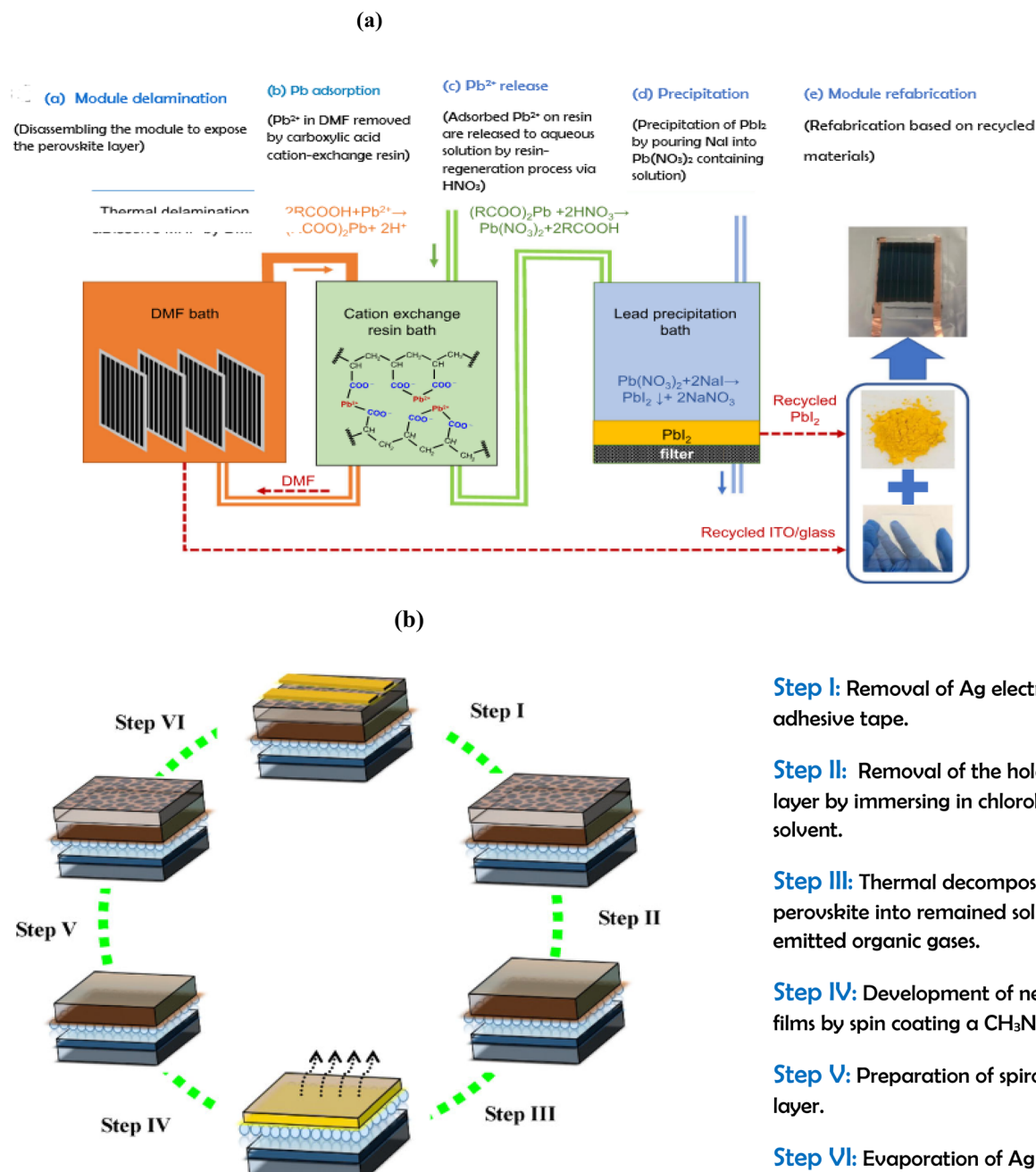


Fig. 8 Lead recovery from perovskites: (a) use of cation-exchange resin (CER) to recycle solar modules<sup>51</sup> and (b) illustration of *in situ* recycling of PbI<sub>2</sub> from PSC and re-preparation of new solar cells.<sup>107</sup>

device is being monitored in real operating conditions (presence of environmental stress, bias, and illumination) as the data is being collected without disrupting module operation.<sup>123</sup> Real-time monitoring of MAPbI<sub>3</sub> modules has been attained through the use of electrochemical sensors, optical spectroscopy, and impedance analysis without interruptions. For instance, Suchan *et al.*<sup>124</sup> employed optical *in situ* monitoring to study how perovskite film formation operates under stress conditions, and reported how optoelectronic characteristics of the perovskite change with time. Similarly, Yuan *et al.*<sup>125</sup> and colleagues applied short-wavelength infra-red holography to

understand how stress-induced defects affect perovskite performance in real-time. Moreover, scientific evidence has demonstrated how real-time monitoring of PV modules can be used to monitor moisture ingress, phase segregation, and ion migration continuously during device operation.<sup>126,127</sup> These studies demonstrate success *in situ* monitoring in real-time when tailoring electronic properties during film growth, tracking how stress defects form, and the time dependence of PV degradation. Real-time monitoring *in situ* may also be extended to various growth recipes and synthesis environments.





Fig. 9 Challenges in recycling of perovskite solar modules.<sup>79</sup>

Another frequently studied approach to Pb recovery is chemical precipitation, where degraded perovskite modules are dissolved in aqueous solutions and reacted with precipitating agents, such as sulfates, phosphates, or carbonates.<sup>15,23</sup> These reagents reduce the soluble  $\text{Pb}^{2+}$  ions to the insoluble  $\text{PbSO}_4$  or  $\text{Pb}_3(\text{PO}_4)_2$  forms, which can be filtered and recovered.<sup>23</sup> This method not only prevents Pb from leaching into the environment but also allows the recovered compounds to be reused in industrial processes. Another promising avenue is the use of solvent extraction and ion-exchange approaches.<sup>128</sup> In this approach, organic solvents or functionalized resins selectively trap  $\text{Pb}^{2+}$  from perovskite waste streams. The resulting bound Pb is strippable and can be recaptured in concentrated form. This method has shown significant recovery efficiencies and

minimised the generation of secondary waste.<sup>128,129</sup> Moreover, ion-exchange resins are reusable and reproducible, making them economically more viable when recycled at scale.<sup>22,110</sup>

Electrochemical recovery is also gaining interest in closing the loop in Pb recovery. With a favourable electrochemical potential,  $\text{Pb}^{2+}$  ions in solution can be reduced and plated out as metallic Pb on the electrode surfaces.<sup>115</sup> This technique not only recovers Pb in a useful metallic form but can also be incorporated into closed-loop recycling networks. Electrochemical recovery is particularly attractive because it can be powered by renewable energy sources, thereby reducing the environmental footprint of perovskite recycling even further.<sup>130</sup> Further to direct recovery, scientists are exploring encapsulation-based recycling systems. Such systems include protective



encapsulation layers and built-in sorbents or scavengers that capture  $\text{Pb}^{2+}$  ions released during degradation. At the end of a module's lifetime, the immobilized Pb encapsulation material can be reclaimed and recycled.<sup>18</sup> This proactive approach reduces the risk of environmental pollution during the solar cell's operational phase.<sup>23</sup> A schematic illustration of strategies for Pb recycling from PSCs is presented in Fig. 10.

Perovskites degrade into volatile organic compounds (VOCs) and non-volatile lead iodide ( $\text{PbI}_2$ ). The VOCs escape into the atmosphere, while  $\text{PbI}_2$  can be recycled by supplementing organic perovskite to restore the perovskite film (Fig. 10(a)). However, this method has limited applicability because it depends on the morphology and crystallinity of the residual  $\text{PbI}_2$ . Thus, the success of this method depends on the initial chemical composition and preparation methods of the perovskites.<sup>131</sup> In solvent extraction, the degraded perovskite is immersed in polar protic solvents, such as 2-propanol, deionised water, ethanol, or methanol, to extract the highly soluble MAI and the low-solubility  $\text{PbI}_2$ . Subsequently, aprotic solvents such as DMF or green solvents, including dialkylamines, butylamine, or methylamine, are added to dissolve the Pb compounds. The use of green solvents is preferred due to DMF's toxicity. While some studies have reported the success of solvent extraction for Pb recovery, this method requires large volumes of solvent and has limited selectivity. Electrochemical deposition has been adopted for all Pb-based devices because it allows recovery of up to 99.8% of Pb when properly dissolved.<sup>110,115</sup> Table 5 presents studies that have proposed recovery methods to mitigate the risk of Pb pollution and promote the recycling of key material components for future perovskites.

Previous studies have developed a closed-loop cycle to recycle lead iodide ( $\text{PbI}_2$ ) harvested from waste organic solvents used in the manufacture of PSCs.<sup>138</sup> This process isolates and purifies the precursor, which is then reused, rather than discarding solvent waste streams that are contaminated with dissolved  $\text{PbI}_2$ . This approach not only reduces the amount of toxic Pb entering the environment but also minimizes the need for virgin Pb resources, providing a clear solution to one of the most pressing sustainability challenges associated with scaling up perovskite technology.<sup>138</sup> Among their findings is the conclusion that the reused  $\text{PbI}_2$  can be used in fresh perovskite films without significant deterioration in device performance. This repurposed material produced perovskite layers with crystallinity, morphology, and optoelectronic properties comparable to those produced with commercial  $\text{PbI}_2$ . A closed-loop system also has economic and environmental advantages. The reuse of  $\text{PbI}_2$  allows manufacturers to not only lower the price of raw materials but also the cost of hazardous waste management.<sup>136,139</sup> The technique also minimises the environmental impact of perovskite production, thereby addressing one of the primary concerns associated with the use of toxic Pb. Accordingly, recycling reduces the risk of Pb leaching into soils and water systems, which is among the greatest challenges to the spread of perovskites in the renewable energy market.<sup>18</sup>

## 7. Applications of AI-powered algorithms in lead leakage monitoring

Machine learning (ML) algorithms (a branch of AI) have transformed the material science landscape, offering the capability

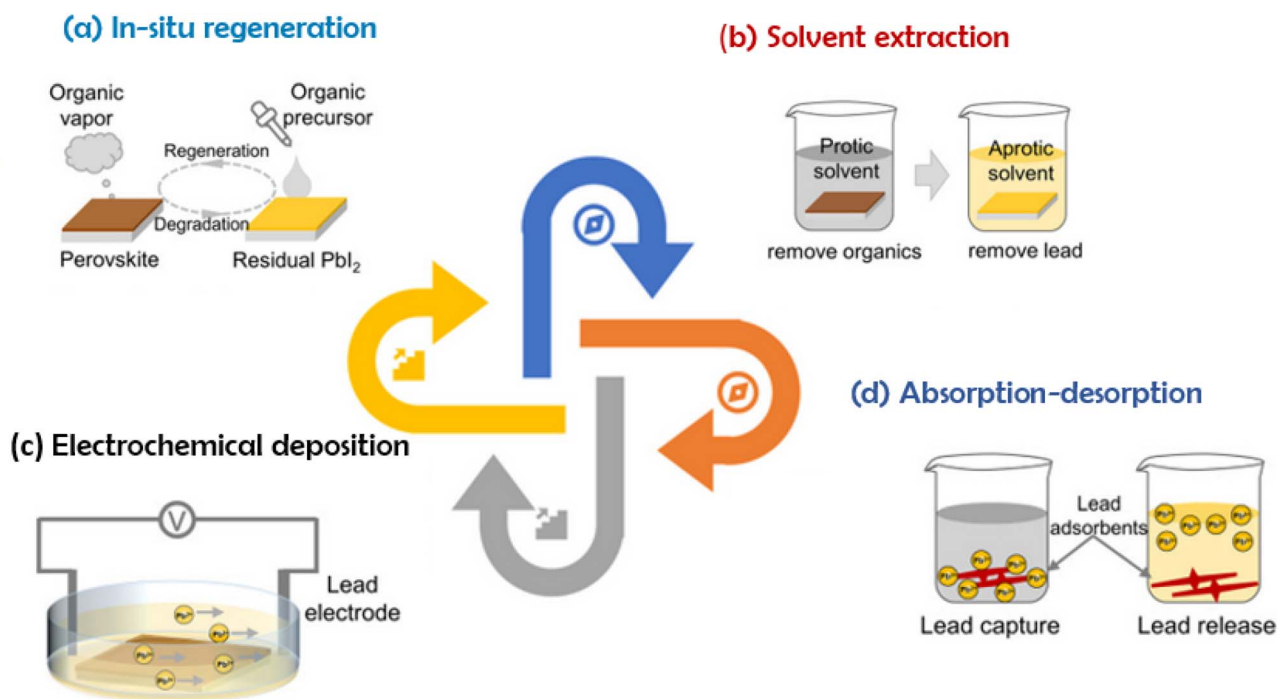


Fig. 10 Lead recovery strategies from lead-based perovskites: (a) *in situ* regeneration, (b) solvent extraction, (c) electrochemical deposition, and (d) adsorption-desorption.<sup>131</sup>



Table 5 Performance of different techniques reported for lead recovery and/or reuse

Method	Lead source	Pb retrieval (%)	Pb recovery (%)	Device efficiency (fresh PbI <sub>2</sub> )	Device efficiency (recycled PbI <sub>2</sub> )	Ref.
Electrochemical	Devices in molten LiCl–KCl perovskite films dissolved in a deep eutectic solvent	>99.8	98	—	—	43
		98.7–99.8	99.8	—	—	115
Ion exchange	Planar TiO <sub>2</sub> devices in DMF	99.99	99.97	16.7	16.5	112
	Pb (NO <sub>3</sub> ) <sub>2</sub> aqueous solution	—	—	19.3	19.0	132
	PbI <sub>2</sub> (aq) from degraded devices	88	96.5	21.0	21.0	133
Solvent extraction/ recrystallisation	PbI <sub>2</sub> from mini modules in DMF	99.6	99.2	21.0	20.5	51
	PbI <sub>2</sub> from carbon-based devices in DM	99.9	95.7	12.2	11.4	113
	Inverted devices in butylamine	—	98.9	17.0	17.0	134
	TiO <sub>2</sub> devices in DMF	—	—	—	13.5	135
	Synthetic solution (TiO <sub>2</sub> , spiro-OMeTAD, PbI <sub>2</sub> , MAI in water)	91.3	—	—	—	136
	Full device in bleaching solution	99.9	100.0	21.0	—	137

to identify degradation pathways, predict material properties, or even propose optimal processing and synthesis conditions.<sup>140</sup> Different from giving data on PV characteristics of PSCs, ML models have been trained on labelled data to elucidate degradation behaviour. Moreover, explainable AI (XAI) is essential in validating recycling processes by determining which variables have the most significant impact on recovery success.<sup>141</sup> This transparency aids regulatory compliance and industry scalability of LPSCs. AI-assisted approaches facilitate the design of a circular manufacturing model in which recovered Pb is recycled and used to fabricate new PSCs, thereby minimizing environmental footprint and material waste.<sup>142</sup> PSCs are sensitive to environmental factors, including humidity, UV radiation, and thermal cycling, and such measures are indicators of one of the major obstacles to long-term stability of PSCs.<sup>81,143</sup> AI methods can mitigate these problems through prediction and diagnosis.<sup>144,145</sup> The neural networks are especially helpful in modelling the complex kinetics of degradation, which allows a scientist not only to estimate how long these devices will last, but also to predict the type of failures that might also occur.<sup>146</sup> This is supplemented by support vector machines, which classify degradation patterns using sensor data, differentiating between reversible and irreversible damage.<sup>147</sup> Visual inspection with convolutional neural networks (CNNs) could identify morphological defects in perovskite films, including pin holes, cracking, and phase segregation.<sup>148</sup> These insights play a key role in quality control and early intervention. This is achievable by learning reinforcement-based dynamic encapsulation systems that adaptively modify barrier properties in dynamically changing environments to enhance device longevity.<sup>148</sup>

AI strategies could reduce development time and costs, paving the way for commercially viable, environmentally responsible PV technologies. PSC technology requires EoL control to mitigate environmental contamination due to Pb and allow sustainable use. AI practice in the field of LPSCs supports predictive maintenance, automated disassembly, and smart recycling decisions, toward circular economy.<sup>149</sup> Support vector machine and machine learning schemes are capable of predicting the performance collapse of a machine based on the data of its operation, enabling timely intervention and Pb

recovery.<sup>150</sup> Explainable AI can be applied to LCA, quantifying the environmental impact of various EoL alternatives to support policy-making and stakeholder engagement.<sup>151</sup> In addition, convolutional neural networks can simplify this step by detecting damaged or contaminated modules *via* visual inspection, thereby improving the efficiency of the recycling pipeline.<sup>152</sup> Through such AI-driven applications, ML algorithms will contribute constructively to the development of sustainable and scalable LPSCs.<sup>151</sup> A summary of various AI techniques that may be applicable to PSC research is presented in Table 6.

Researchers at the University of Washington developed physicochemical ML models to predict the lifetime of MAPbI<sub>3</sub>-based solar cells.<sup>146</sup> The research team further utilised various regression algorithms to predict device stability, employing Lasso regressions. Notably, the findings of this research group emphasised the importance of AI in quantifying the parameters that improve operational stability.<sup>146</sup> AI has also been applied to accelerated ageing experiments, where perovskite modules were exposed to simulated stress conditions, such as high humidity, UV radiation, and high temperatures.<sup>157</sup> Trained ML models based on these datasets can extrapolate long-term degradation trends to short-term experiments, reducing the time and cost of stability tests by many orders of magnitude. This technique can be particularly beneficial for estimating the extent of Pb leakage under extreme weather conditions that are difficult to replicate in a laboratory yet vital to practical applications.<sup>58</sup> More so, AI can help with automated defect detection in perovskite films.<sup>158</sup> Computer vision algorithms trained on microscopy images can detect microcracks, pinholes, and phase-segregation patterns that often precede Pb leakage. When installed on manufacturing lines, these systems can provide real-time quality control, enabling defective modules to be identified and corrected before being fabricated. This not only improves the reliability of the devices but also reduces the risk of faulty products polluting the environment.<sup>33</sup>

Another prospective application of AI in this field is integrating predictive modelling with real-time sensor data. By combining information from fluorescence sensors, electrochemical measurements, and ICP-MS, it is possible to identify



Table 6 Emerging AI techniques for potential applications of AI in perovskite solar research

AI technique	Application area	Advantages	Limitations	Ref.
Machine learning	Material screening and composition prediction	Rapid identification of stable, high-efficiency materials reduces experimental workload	Requires large, high-quality datasets; may over fit to known materials	153
Neural networks	Modelling degradation kinetics	Model nonlinear relationships between fabrication parameters and PCE; adaptable to new data	Often lacks interpretability; sensitive to noise in training data	154
Explainable AI	Manufacturing optimization, material recovery, and decision support	Provides insights into model decisions; improves trust and transparency	Still emerging in materials science; limited toolkits	155
Support vector machines	Classification of degradation patterns and failure modes	Effective for small datasets; robust to overfitting	Less effective for large, noisy datasets; limited scalability	156
Convolutional neural networks	Image-based defect detection in perovskite films	High accuracy in visual inspection enables real-time quality control	Requires labeled image datasets; computationally demanding	148

early indicators of Pb leakage before it becomes harmful. Such predictive frameworks enable operators to implement proactive measures, such as module replacement or encapsulation strengthening, which reduce environmental contamination risks.<sup>50,159</sup> Joji *et al.*<sup>42</sup> utilised a biomimetic sensing moiety to detect Pb ions and amino acids in water leaked from LPSCs. They demonstrated the use of pulse voltammetry, utilising a zeolitic imidazolate framework-nitrogen-doped (ZIF-N) as the sensing element. These studies have demonstrated the potential of integrating AI predictive modelling with real-time sensor data in controlling Pb leakage from PSCs. Another notable contribution of AI is in the extraction of characteristics from complex degradation datasets. The mechanisms that result in the degradation of PSCs are multifaceted and encompass multiple processes that interact with one another, including ion transportation, water ingress, and thermal stress.<sup>104,160</sup> Traditional statistical methods often overlook these nonlinear interactions. Nevertheless, deep learning models can process large multidimensional datasets to reveal latent relationships between environmental stressors and Pb release. This enables researchers to determine the most feeble degradation triggers and develop more robust device architectures.<sup>50</sup>

There are existing studies have successfully applied AI algorithms like ML to forecast new solar cell designs with strong performance and mechanical stability. ML-assisted designs have been employed to optimize defect tolerance and spectral response of perovskite photodetectors.<sup>161</sup> This highlights the huge prospects of AI in analysing complex PSCs behaviour relevant to the MAPbI<sub>3</sub> degradation pathways. Electrochemical techniques have also been combined with AI algorithms to create AI-assisted sensors, which have enhanced the selectivity and sensitivity of Pb<sup>2+</sup> in soil and water systems. Design and development of PSCs have also utilized AI to accelerate the discovery and validation of experimental and theoretical data.<sup>162</sup> However, some approaches are still speculative. For instance, whereas there exist proposals to use AI algorithms in predicting degradation due to mechanical stress, UV exposure, and

humidity, there exist no industrially validated datasets to train robust AI models. The idea of using AI-based Internet of Things (IoT) sensor networks to monitor real-time Pb degradation is still at infancy since there exist no prototypes of portable sensors that have been integrated in autonomous self-learning networks. Secondly, no empirical data exists to support the use of AI in governance integration and policy frameworks, particularly in alignment with JT frameworks.

## 8. Life cycle assessment of lead-based perovskite solar cells

LCA of PSCs has been employed to examine the material composition of solar cell devices, particularly the amount of Pb in commonly used halide perovskites. Currently, the densities and molecular weights of formamidinium lead iodide (FAPbI<sub>3</sub>, 4.10 g cm<sup>-3</sup>, 636 g mol<sup>-1</sup>), methylammonium lead bromide (MAPbBr<sub>3</sub>, 3.83 g cm<sup>-3</sup>, 482 g mol<sup>-1</sup>), and (MAPbI<sub>3</sub>, 4.09 g cm<sup>-3</sup>, 619.98 g mol<sup>-1</sup>) are typically employed to assess Pb concentration.<sup>163</sup> These values act as a baseline against which the potential environmental risks of Pb leakage can be evaluated when producing, using, and disposing of perovskite-based devices.<sup>31</sup> Among the most problematic aspects of the life cycle of PSCs is that they are prone to degradation under real-world operating conditions.<sup>18</sup> The breakdown of perovskite films is also susceptible to degradation from various factors, including exposure to oxygen, moisture, heat, light, and even electric fields, which can reduce their stability and lifespan.<sup>18</sup> These stressors are largely unavoidable in operation and therefore constitute a significant barrier to commercialising perovskite photovoltaics. Not only does degradation impact efficiency, but it also raises serious concerns about the release of toxic substances, such as Pb, into the environment.<sup>103</sup>

The purpose of LCA is to conduct a systematic evaluation of the environmental impact of PSCs within a lifecycle framework, encompassing the mining of raw materials, device manufacturing, operation, and disposal.<sup>164</sup> This holistic



approach enables researchers to identify the stages at which environmental burdens are most critical and recommend effective mitigation measures. LPSCs, despite their high-power conversion efficiencies, must be evaluated against conventional silicon solar cells, which are more stable though require energy-intensive manufacturing.<sup>164</sup> Comparative LCA studies have shown that PSCs generally have shorter energy payback times and lower greenhouse gas emissions than silicon-based technologies.<sup>97</sup> However, the presence of Pb is a major drawback, where improper excavation or gradual wear can result in soil and water contamination. Researchers are therefore exploring Pb-free alternatives, such as tin-based perovskites, albeit with lower efficiency and stability challenges.<sup>104</sup> The sustainability analysis of perovskite photovoltaics remains centred on the performance-environmental safety trade-off.<sup>31</sup> The introduction of LCA into the perovskite field provides a framework that guides material development, device design, and recycling decisions. By quantifying the environmental impact at each stage of the product life cycle, stakeholders can make knowledge-based decisions to increase production without ecological degradation.<sup>103</sup> The future will require improvements in encapsulation measures, recycling techniques, and the development of less toxic materials to ensure that PSCs can make a positive contribution to the global transition to renewable energy.<sup>14,18,165</sup>

Among the documented comparative LCA of PSCs, scientists at Chalmers University of Technology compared the environmental performance of perovskite modules with that of traditional silicon solar cells.<sup>166</sup> The study found that perovskites also had a significantly shorter energy payback time because they were prepared as low-temperature solutions. However, their findings also highlighted that the instability of perovskites and the potential for releasing Pb during degradation posed environmental hazards and, therefore, are not environmentally sustainable.<sup>166</sup> An extensive case study by Khan<sup>167</sup> at the German Aerospace Centre (DLR) explored the LCA of future perovskite/silicon tandem solar cells. The study noted that tandem designs could reduce the overall carbon footprint of photovoltaics by improving efficiency and reducing the material volume per unit of electricity generated. The experiment, nonetheless, noted that environmental benefits were highly dependent on the stability of the perovskite layer because frequent replacement or degradation of the layer would offset the gains.<sup>167</sup>

## 9. Just transition to clean energy

Just transitions (JT) reflect the recognition that the transition to renewable energy is to mitigate greenhouse gas emissions and prioritize equity, justice, and community welfare. Energy justice is multidimensional, encompassing environmental health, community participation, equitable access, and labour rights.<sup>168</sup> LPSCs containing toxic Pb raise serious ethical concerns about the trade-off between technological promise and etiological risks, owing to their strong potential to deliver high efficiency and stability.<sup>38</sup> They offer a pathway to the democratization of solar energy, but they raise significant concerns regarding toxicity, environmental equity, and the uneven distribution of

burdens and benefits. The risk of Pb leakage during the manufacturing, use, or disposal of perovskites remains unresolved despite ongoing research. Whereas efficiency, stability, and scale improvements dominate emerging scientific reports, and toxicity is occasionally addressed as a secondary concern through encapsulation or recycling.<sup>169</sup> This underscores the tendency of industrial pioneers to prioritize performance metrics over social and environmental problems. Communities around manufacturing and waste-dumping sites also experience unprecedented consequences of new technologies.<sup>170</sup> In cases of LPSCs, such communities can be disproportionately exposed to dangerous materials and the far-reaching implications of industrial effluents.<sup>171</sup> Without proactive measures such as recycling mandates, the deployment of LPSCs risks reproducing the injustices of past energy systems, where the rich minority would hold the gains and the burdens would fall on vulnerable communities.

Theoretically, low-cost PSCs could democratize solar adoption by reducing barriers to entry.<sup>172</sup> However, with rapid advancement of LPSCs is envisaged to accelerate decarbonisation, critical issues, such as the use of toxic materials, remain uncertain. The rush to deploy LPSCs without appropriate safeguards creates new injustices to communities exposed to Pb pollution. To ensure equitable outcomes, participatory governance should involve communities in discussions about siting, production, and waste management.<sup>173</sup> This would ensure that the benefits of LPSC deployment, such as improved access to clean, secure, and affordable energy, are distributed equally. There should also be transparent monitoring of emissions and strict recycling protocols to mitigate Pb leaching, with these protocols implemented in ways that are accountable and accessible to communities.

Marginalized groups such as rural communities, the indigenous population, and low-income households should be prioritized in expanding access to solar energy to mitigate existing inequalities.<sup>174</sup> Previous studies have also shown that policies and regulations can serve as mediators in the development of risk management actions of LPSCs guided by justice principles. Strong governance frameworks, including safe material management, recycling mandates, and international standards, are essential for addressing inequitable harm.<sup>175</sup> There is still a need for interdisciplinary research that bridges the gap between social justice and materials science, ensuring that innovations in PSCs are driven by equity and justice considerations. JT is not only about decarbonisation but also about ensuring that societies are more inclusive, equitable, resilient, and secure while embracing green energy transition.<sup>170</sup>

### 9.1. Relevant laws and legislation

Research laboratories and several companies are advancing LPSCs toward commercialisation; now, relevant laws and regulations need to be implemented to reduce and restrict Pb pollution. The highest-performing and most promising perovskite solar panels to be commercialised contain a highly toxic Pb, which can pose a potential risk to human health and the environment, as Pb<sup>2+</sup> are soluble in water and can be absorbed



into biological systems.<sup>34</sup> Once a Pb particle is inside the body, it remains in soft tissues, and with continued exposure, it can be absorbed into the teeth and bones, potentially reducing its half-life to 20–30 years.<sup>176</sup> The Restriction of Hazardous Substances (RoHS) and the United States Resource Conservation and Recovery Act (RCRA) both aim to reduce the risks associated with the use of hazardous materials and with disposal by regulating the transportation, generation, treatment, and disposal of hazardous waste.<sup>177</sup> According to the EU, the RoHS directive primarily prevents the distribution of potentially hazardous commercial electrical and electronic (EE) products by restricting the use of hazardous substances and evaluating them on a per-weight basis. Here, the tolerated weight concentration limit for Pb in PSCs is 1000 mg kg<sup>-1</sup> for the EU market.<sup>177</sup> Moody *et al.*<sup>177</sup> reported that the leaching of perovskite PVs poses a higher risk to environmental health than the Pb content itself, potentially endangering human life. The National Ambient Air Quality Standards (NAAQS) regulate the air concentrations of ozone, nitrogen dioxide, sulfur dioxide, carbon(IV) oxide, and Pb. The maximum safe level of Pb in ambient air is 0.15 µg m<sup>-3</sup>, based on a three-month average.<sup>178</sup>

Accordingly, the legal framework for human health integrates specific global standards. For instance, the European Union (EU) has set standards and restrictions on the use of sludge containing metals, including Pb. EU limits Pb concentration in “homogenous materials” to 0.1% by weight.<sup>179</sup> With respect to this, solar modules, “intended to be used in a system that is designed, assembled and installed by professionals for permanent use at a defined location”, are exempted from this restriction. Nevertheless, this legislation does not apply to devices embedded in portable systems or consumer electronics; specific legislation regulating immobilisation will be needed in the future. According to the World Health Organisation (WHO), the total Pb content in drinking water should not exceed 10 µg L<sup>-1</sup>. In China, the upper limit of Pb content in agricultural soils is 250 mg kg<sup>-1</sup> to limit human exposure. Additionally, the United Nations (UN) Food and Agriculture Organisation (FAO) has established maximum Pb concentrations in canned food and beverages at 250 mg kg<sup>-1</sup> and 150 mg kg<sup>-1</sup>, respectively.<sup>180</sup> Elsewhere, the United States has set the safe-to-use Pb level at 5 µg L<sup>-1</sup>, with the goal of ensuring zero Pb content in drinking water.<sup>180</sup> Also, the Centres for Disease Control (CDC) has set the limit blood Pb concentration of 3.5 µg dL<sup>-1</sup>.<sup>181</sup>

The Waste Electrical and Electronic Equipment (WEEE) directive involves large quantities of metals that can be isolated, recovered, and recycled, thereby providing substantial environmental benefits by decongesting landfills of potentially hazardous materials and reducing the risk of neurological disorders and cancer.<sup>182</sup> Photovoltaics that can be reused, repaired, upgraded, remanufactured, disassembled, and efficiently recycled would have lower EoL costs, leading to a competitive Levelized Cost of Energy (LCOE) advantage.<sup>183</sup> On the other hand, the RoHS directive limits Pb content to ≤0.1 wt% in homogeneous materials (*i.e.*, materials with uniform composition throughout).<sup>183</sup> Prior studies have shown that mass roll-to-roll (R2R) manufacturing could substantially reduce the environmental footprint per watt of electricity

production.<sup>167</sup> Research has also highlighted that without efficient recycling strategies, the toxicity of Pb-containing waste may pose a severe ecological hazard in the long term.<sup>167</sup> Remarkably, a comparative LCA of Pb-based and Pb-free perovskites revealed that whereas Sn-based perovskites may reduce toxicity concerns, they do not compete with Pb-based perovskites in terms of efficiency and stability.<sup>169</sup> However, the net environmental impact of tin-based devices may be higher due to shorter life and lower energy efficiency. Thus, improved encapsulation and recycling of LPSCs could be a more sustainable approach than switching to less efficient Pb-free perovskites.<sup>166</sup>

## 10. Future perspectives

Integration of Pb detection and monitoring techniques with JT principles into the deployment of PSCs remains a fundamental gap that demands attention for future research. Although detection and monitoring techniques have made remarkable advancements, they are restricted to laboratory-based demonstrations, which do not represent real-world conditions.<sup>184</sup> In practice, PSCs are subjected to mechanical stress, temperature variations, and humidity.<sup>38</sup> Therefore, without rigorous field validation, Pb leaching may continue until public trust and environmental safety are undermined. Moreover, the available ML algorithms data are fragmented, and there are limited generalizability and reproducibility of predictive models towards PSCs. This is a technological hurdle that hinders the development of globally acceptable monitoring systems. Therefore, additional research must focus on developing open-access datasets, which will help benchmark and expedite the development of universally acceptable monitoring systems. Accordingly, the shared resources will enable model frequency, support disassembly and recycling strategies.

Fundamental studies on encapsulation engineering have underscored them as primary mitigation strategies to address Pb leakage. However, this approach fails to resolve issues such as EoL management, circular economy strategies, policy integration, recycling, safe disposal, and socio-technical considerations.<sup>38</sup> Future investigations should focus on bridging the gap of justice concerns and technological detection methods. Encapsulation mechanisms that adapt to the environment should be developed. Additionally, participatory monitoring frameworks should involve affected communities in decision-making about waste management, production and siting to ensure adherence to policies like WHO drinking water limit and CDC lead threshold of the blood. This will make sure that technical innovation connects to equitable governance. Sustainability and performance principles should also guide the selection of materials used in PSCs.<sup>185</sup>

Whereas transition to lead-free PSC has been reported in prior studies as a solution to minimize the Pb leaching of PSCs, Pb-free alternatives have other analytic issues that need considerations.<sup>185</sup> Sn-based devices, including Sn-based devices, are prone to instabilities and lower efficiency since the oxidation of Sn<sup>2+</sup> to Sn<sup>4+</sup> is rapid. In view of this, the focus shifts to monitoring Pb<sup>2+</sup> mobilization to oxidation-state



transitions in Sn. This implies that instead of using the already optimized techniques such as ICP-MS, *in situ* methods such as X-ray absorption and spectrochemical probes of redox systems must be improved. Additionally-Bi-based PSCs, can leach various species into the environment due to environmental degradation factors. While Pb-free alternatives are considered less toxic, they pose introduce scientific difficulties in terms of detection and quantification of  $\text{Sb}^{3+}$ ,  $\text{Bi}^{3+}$ , and other leached, soluble PSCs species. Therefore, the challenge of Pb toxicity evolves to multi-element quantification and stability assessment. Furthermore, the transition to lead-free PSCs presents a paradigm shift regarding the application of the monitoring strategies.<sup>104</sup> In the PSC settings, the ICP-MS is considered a gold standard, yet the focus will be on monitoring and quantification methods that prioritize field-applications and accessibility. This means that simple electrochemical instruments such as spectroscopic probes and electrochemical sensors that measure oxidation dynamics in real time will become prominent. The monitoring will also shift to less toxicology-based and more durability-based, and scientists will anticipate for materials that do not introduce unforeseen risks.<sup>104</sup> Eventually, the shift to Pb-free will involve adaptive, cost-efficient, and inclusive technologies that can track the environmental interactions and degradation pathways of the modules.

## 11. Conclusions

In this review, we have provided a concise discussion on the prospects of perovskites, degradation pathways of  $\text{MAPbI}_3$ -based devices, the environmental hazards associated with Pb leakage, Pb leakage detection strategies, including potential integration of AI to monitor Pb leakage, strategies for Pb immobilisation, recycling methods, and end-of-life management of decommissioned modules. Also, the balance between JT in embracing clean energy and the deployment of LPSCs among communities has been extensively discussed. Currently, perovskite solar technology is a leading candidate in the solar energy market; however, industrial advancement remains hindered by challenges in upscaling and stability. Encapsulation engineering strategies have been tested to address concerns about oxygen- and water-related degradation; nonetheless, inherent challenges related to light and thermal effects remain unresolved. To be able to compete with the widely deployed and most mature solar technology, industrial pioneers of perovskites must strive to narrow the efficiency gap between laboratory- and commercial-scale devices. By adopting strategies such as green solvents, device recycling, and encapsulation, the environmental impact of perovskites can be significantly reduced. Accordingly, AI offers a transformative pathway that not only accelerates predictive modelling and design strategies but also enables more effective monitoring of perovskite degradation. Ultimately, AI will transform the perovskite technology landscape, as AI-guided perovskite technologies are key to transitioning to sustainable solar power. As perovskite technology nears commercialisation, its successful deployment hinges on the use of green precursors to enable safer, more

sustainable fabrication and recycling strategies. While Pb-free perovskite could offer new end-of-life management platforms, these devices are plagued by low efficiencies. Recent advances in Pb sequestration, particularly in external and internal encapsulation strategies for Pb capture and improved mechanical stability, offer promise for deployment and just transition protocols. However, recycling perovskites poses enormous challenges related to device stability and recycled device efficiency. Serious research is underway to develop a potential paradigm shift toward Pb-free perovskites to reduce health and environmental risks associated with LPSCs. Consequently, Pb-free perovskites will have different material composition, including the active layer, ETLs, and HTLs, offering the scientific community opportunities for recycling and environmental sustainability. The future outlook for perovskites is that additional research should focus on green, sustainable recycling protocols. Bearing this in mind, research on perovskites should not be restricted to one family (Pb-based devices), but also include new materials such as non-perovskites and chalcogenide-based perovskites with novel structures that offer bankability in terms of stability and optoelectronic properties. Future research should also focus on other applications of perovskite, such as light-emitting diodes (LEDs), detectors, lasers, and memory devices.

## Conflicts of interest

The authors declare no conflicts of interest.

## Consent for publication

This article has the consent of all the authors.

## Data availability

No new data were generated, as this is a review paper. Secondary research data has been used.

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