

Drawback and Improvements of Current Perovskite Solar Cells

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Abstract. The concept of "sustainable solar cells" encompasses the dual objectives of promoting human health and advancing sustainable societal progress. Perovskite solar cells (PSCs) have garnered significant attention over the years as promising contenders, recently reaching power conversion efficiencies (PCEs) exceeding 25%. Nonetheless, a majority of the primary materials in PSC production are recognized as hazardous by multiple environmental bodies. While there have been initial efforts, both chemically and physically, to develop less toxic PSCs, the PCE of these environmentally-friendly variants remains subpar when compared to their traditional counterparts. Hence, the balance between toxicity and efficiency has emerged as a pivotal concern for the PSC market. Viewing this through a lens of sustainability, it becomes evident why PSCs have become a dominant choice for sustainable solar technology. The subsequent focus should be on addressing the limitations—mainly toxicity and stability—associated with PSCs. The toxicity inherent in PSCs is largely attributed to the inclusion of heavy metals, such as lead, and halogens in its molecular composition. Concurrently, stability issues stand as significant barriers to the large-scale manufacturing of PSCs. Thus, pinpointing the equilibrium between toxicity and efficiency is vital for the successful market integration of PSCs. Finally, potential solutions to mitigate these shortcomings will be outlined.

Keywords: Interfaces, toxicity, perovskites, solar cells, stability.

1. Introduction

In addressing the environmental concerns arising from combustion-based energy production, photovoltaic (PV) technologies emerge as pivotal contributors to a sustainable and clean energy landscape. Specifically, perovskites, characterized by their prominent light absorption coefficients, elevated carrier mobility, and amenability to cost-effective production, have garnered substantial interest in the realm of solar energy over the previous ten years. Perovskite modules have achieved PCE certifications of 20.2% for 20 cm² and an impressive 29.5% when integrated with silicon in tandem structures. Owing to this exemplary efficacy, PSCs hold vast potential for extensive applications. Moreover, the tunable band gaps and fabrication ease of perovskite solar modules suggest their potential synergy with silicon PV technologies, aiming for superior market conversion efficiencies [1]. Notably, PSCs are poised to outperform traditional power sources. The inherent high absorption coefficient of perovskites paves the way for the creation of ultra-efficient solar cells with slender absorption layers, positioning them as prime candidates for semi-transparent architectural solar applications, coupled with promising flexibility and suitability for wearable electronics. Anticipation runs high for the upscaling of PSC production, which is foreseen as a catalyst for worldwide decarbonization efforts in the imminent future. This momentum is underscored by the surge of PSC-oriented startups transitioning from academic research settings to industrial platforms, setting the stage for expansive applications.

While the exceptional characteristics of perovskites suggest a promising horizon for PSCs, sustainable usage faces considerable challenges that remain unresolved (Fig. 1) [2]. In the context of stability surpassing commercial benchmarks, PSCs present significant shortcomings. The susceptibility of these cells to light arises from their fragile hydrogen bonds, which, upon exposure, fracture, prompting halogen movement into the perovskites. Moreover, the organic elements within perovskites exhibit reduced thermal stability, leading to decomposition at functional temperatures. Environmental factors such as humidity and oxygen further hasten the deterioration of perovskites.

Prominently, contemporary efforts have centered on refining the perovskite architecture through element doping and ion replacement, with objectives to amplify its luminescence and enhance thermal resilience. In tandem, approaches encompassing the integration of hydrophobic interlayers, modifications to electrodes, and fortified encapsulation are pursued to protect perovskites from external threats, including humidity and oxygen. By employing tactics like compositional tailoring, structural fine-tuning, and sophisticated encasement, a significant alleviation of their stability concerns has been observed.



Figure 1. Limitations in Advancing Sustainable PSCs.

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A predominant challenge for the viability of sustainable PSC pertains to its inherent toxicity. Addressing stability and manufacturing challenges of PSC isn't the sole issue; the toxic nature of PSC could impede its widespread adoption given that substantial photovoltaic modules are imperative for consistent energy provision. It is thus crucial for the production and operation of perovskite solar modules to adhere to environmental standards to effectively mitigate ecological concerns and pave the path for sustainable development. Regrettably, the large-scale production of PSC often involves the use of numerous harmful substances [3]. Moreover, OIHP elements infuse harmful organic ions and halides. Notably, the dominant efficient PSC technologies predominantly utilize perovskite, characterized by lead ions situated at the B site. The accumulation of Pb^{2+} in our ecosystems and food webs can lead to detrimental impacts on various human systems, including hematopoietic, neurological, reproductive, and metabolic systems. Beyond the adverse effects of lead, the extensive use of organic solvents during the dissolution phase stands as a notable source of toxicity. While these solvents prove effective in curbing production expenses, they bear the potential to contaminate terrestrial and aquatic ecosystems. For instance, N, N-dimethylformamide (DMF), a principal solvent for crafting perovskite precursors, manifests acute toxic impacts on the skin, mucous membranes, and internal organs. Prolonged exposure to DMF could adversely impact the respiratory, nervous, hepatic, and renal systems. It's worth noting that a majority of the primary ingredients used in CCS production are categorized as hazardous by several environmental bodies. Hence, forthcoming research endeavors should pivot towards diminishing the toxicity of PSC, all while preserving its efficacy.

2. Advantages and Disadvantages of Perovskite Cells

2.1. Advantages

For a long time, silicon material has been regarded as the basic raw material of the photovoltaic industry. There has been a saying in the industry that "those who get silicon material win the world". Based on silicon material, the traditional crystalline silicon battery is obtained. The current TOPCON battery and heterojunction battery are all traditional crystalline silicon cells, which are the second-generation photovoltaic cell technology. Perovskite battery is the representative of the third generation of non-silicon thin film battery. Compared with the second generation, perovskite battery has obvious advantages, such as high conversion efficiency and low cost. In the context of expanding power scales and the inherent constraints of silicon-based materials, the primary avenue for advancing photovoltaic cells lies in enhancing their conversion efficiency. Established crystalline silicon cells approach their envisaged efficiency ceiling of 29.4%. In contrast, single junction perovskite cells possess a conceivable peak efficiency reaching 31%. Moreover, multi-junction perovskite cells boast a staggering theoretical limit of 45% conversion efficiency. This surpasses the efficiency of crystalline silicon cells significantly, underscoring the growing interest in perovskite solar cell research and development. Perovskite battery has low investment cost, low production cost, large cost reduction space, high production efficiency and sufficient competitive advantage. The cost advantage of single junction perovskite battery is obvious, and the investment required to achieve 1GW capacity is only about 500million yuan, which is about 1/2 of the production cost of the same level crystalline silicon battery; The consumption of raw materials is small, accounting for only 5%; The production is vertically integrated and takes less time than that of crystalline silicon batteries. The 100MW single junction perovskite production line takes only 45 minutes from raw materials to component molding; The production of crystalline silicon batteries requires a high temperature of more than 1700 degrees, while the maximum temperature of perovskite batteries from beginning to end will not exceed 150 degrees. The purity requirement is low, and the energy consumption per watt is only 1/10 of that of crystalline silicon; The investment per unit capacity of perovskite battery in mature stage is 1/2 of that of crystalline silicon battery, and the actual power generation efficiency is higher than that of crystalline silicon battery. The stack technology can improve the photoelectric conversion efficiency. The laboratory efficiency of perovskite and crystalline silicon stack cells at both ends is more than 31%; The theoretical efficiency of the two-end stacked battery can reach 45%, which is much higher than the s-q limit efficiency of the single junction battery of 33% and the laboratory efficiency record of the single junction battery of 25.7%.

Perovskite solar cells are characterized by a concise production procedure, distinguishing them from other photovoltaic technologies. A notable benefit of perovskites is their cost-efficiency. In their study, Song et al. [4] formulated a comprehensive cost model from a bottom-up approach to assess the financial implications of perovskite solar cell modules. These modules are crafted utilizing economical materials and methodologies. A depiction of their production, which covers an expansive surface area via a systematic low-temperature deposition method [5]. The projected manufacturing expenses ranged from \$5.5 to \$31.7/m². This estimation breaks down into the actual perovskite cell operation costs (\$1.2 to \$6.8/m²) and the associated costs of module components (\$4.3 to \$24.9/m²) - elements like glass and frames are included in this bracket. The perovskite production is marked by limited stages and commendable efficiency.

2.2. Disadvantages

2.2.1. Toxicity

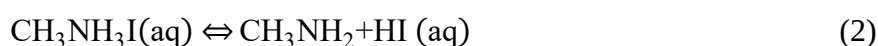
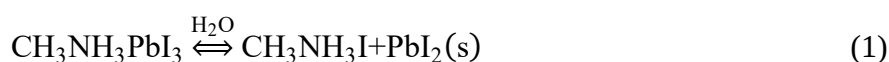
In contrast to the diverse selections available at site A in oihp, the majority of sophisticated PSCs prefer PB at site B. Lead, identified as a substantial societal menace, is notably more deleterious than the A-site cation in PSCs. When introduced to air or water, the risks of acute and prolonged toxic effects on humans are broad. Contamination by lead can alter genetic material, induce neurotoxic effects, manifest fetal toxicity during gestation or breastfeeding, and harm the kidneys, hematopoiesis,

and the immune system. Children below the age of 5 and expectant mothers are particularly susceptible to lead's adverse effects. Accumulated lead ions can impair the nervous system of children, particularly those with an underdeveloped blood-brain barrier. Diminished blood lead concentrations can result in reduced cognitive capabilities in children, and expecting mothers might experience miscarriages, stillbirths, premature deliveries, or congenital anomalies. Moreover, protracted exposure to lead heightens cancer susceptibility. Consequently, IARC categorized lead as a potential carcinogenic substance for humans. Due to its detrimental impacts, there are widespread regulations restricting lead's presence in everyday commodities. The EU directive 2002/95/etc. mandates that "new electronic and electrical devices introduced in the market must be devoid of elements such as lead, mercury, and cadmium".

By 2011, it was suggested that PV modules ensuring a lead lifecycle could be an exception. Nevertheless, the unstable calcium titanium residue in PSC is prone to breakdown, yielding lead derivatives. Concurrently, the lead KSP is exponentially greater, by 29 orders of magnitude, compared to the previous generation of ecologically debated solar cells, like CdTe, signifying its heightened water solubility. This can consequently contaminate the ecological systems. In essence, the concerns associated with lead-infused perovskites have markedly hindered the commercial prospects of PSCs [6].

2.2.2. Solvent extraction

The degradation of perovskite films can be attributed to four primary determinants: the presence of oxygen and moisture, exposure to ultraviolet (UV) rays, the treatment with specific solutions, and the influence of thermal effects [7]. A sequential set of reactions unfolds during the catalytic breakdown of water in the calcium titanium deposit (equations (1)-(4)).



Numerous studies have highlighted water as a driving force behind the permanent degradation of perovskite materials. Frost and colleagues have illustratively detailed the potential decomposition process of these materials, as presented in Fig. 2 [8]. The depiction verifies that both HI and Ma are soluble in water. The persistent deterioration of the calcium titanate layer compromises the lifespan of photovoltaic cells. Furthermore, the properties of the emerging by-products contribute to the intricacy of the problem. As depicted in Fig. 2, one such by-product of the reaction, which exhibits water solubility [9, 10]. The degradation by-products in the installed module can potentially pose significant ecotoxicological threats to the surrounding environment.

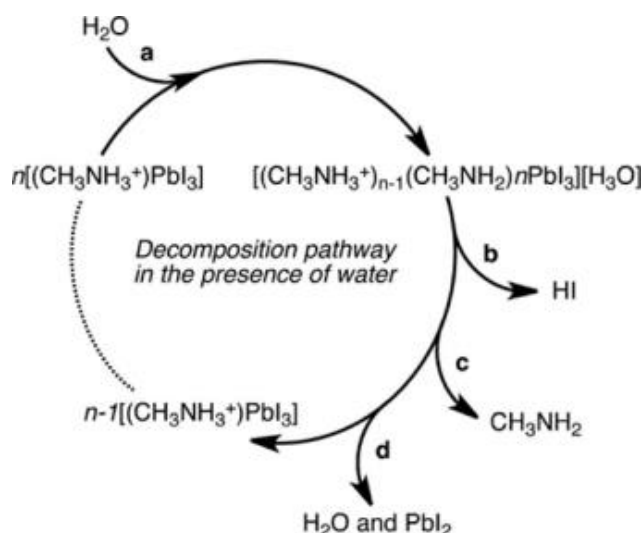


Figure 2. Suggested Disintegration Route of $\text{CH}_3\text{NH}_3\text{PbI}_3$ when Exposed to a Water Molecule. Notably, the predominant outcome of this route is PbI_2 . <https://pubs.acs.org/doi/10.1021/nl500390f>

Established solar cell technologies, including perovskite solar cells, often display susceptibility to ultraviolet radiation-induced degradation. Central to the high efficacy of certain perovskite solar cells highlighted in prior research is the incorporation of the TiO_2 electron transport layer. The architecture of devices utilizing this layer traces back to DSSC, as illustrated by sources such as Lettens et al. Through their investigations, it was discerned that the TiO_2 layer within perovskite solar cells faces degradation due to UV exposure. This inference emerged from the evaluation of a 5-hour efficiency diminution trajectory for devices in varying conditions: encapsulated versus non-encapsulated and with or without UV protection, all under 1 sun am 1.5g lighting. Intriguingly, the data revealed that encapsulated devices experienced a steeper drop in efficiency compared to those not encapsulated.

3. Improvement

3.1. Balance Toxicity and Stability

In pursuit of an optimal solution, the objective is to substitute lead while preserving the significant efficiency inherent to PSC. Various studies indicate that lead ions in perovskite may be exchanged with dimensional equivalents or heteroallene elements that span both low and high spectra. Potential replacements encompass IVA elements, transition metals, and alkaline earth metals, which are ideal for bivalent substitution. Nonetheless, a sizable portion of these proposed materials manifest undesirable band structures, characterized by features like pronounced local band edges, profound states, and overly expansive band gaps. As noted in the research conducted by M. Philip and colleagues, out of 248 potential compounds, only 25 were meticulously assessed to determine their suitability for B-site substitution. Their selection hinged on a dual-criteria framework: the inherent stability of these compounds within the perovskite matrix and the nature of their band gaps. It's pivotal to note that elements like cadmium and mercury were excluded from consideration due to their harmful nature. Moreover, elements such as Ga, In, V, and Ge, despite their potential, are costly and do not deliver superior performance. A pivotal criterion for any suitable replacement is that it possesses an apt band gap ranging from 0.9 to 1.7 eV, alongside a diminished effective electron mass, positioning it as a viable alternative to Pb. Devices utilizing other valence substitution elements, notably Bi and Sb, exhibit an energy conversion efficiency that barely surpasses 3%, a figure considerably beneath the acceptable threshold.

Beyond ion substitution, another pragmatic approach entails the tangible reduction in lead usage, striking a balance between performance and ecological concerns. One such method involves adopting a svelte titanite layer in lieu of the conventional quasicrystal that predominantly absorbs the photon μM layer. Owing to the pronounced absorption coefficient, the device's PCE sustains up to 96% of

its peak capacity, even when the thickness of the calcite layer is diminished to merely a third of its original measure. Such a reduction in layer thickness inherently reduces the lead concentration. Furthermore, ultra-thin layers of calcium titanium can be synergistically integrated with pliable substrates and slender electrodes, heralding a plethora of novel uses, including but not limited to, semi-transparent windows and agile PSCs. This approach is a testament to the potential of redox reactions in enhancing device performance.

3.2. Industrial Treatment for Lead Contamination

Addressing lead contamination is governed by recognized industrial protocols. Numerous strategies have been devised to handle lead ions, depending on the specific situation. These strategies predominantly fall under three categories: physical, chemical, and biological techniques. For instance, when dealing with lead-tainted soil, one could resort to physical solutions such as soil replacement, containment, or thermal interventions. Chemical methods encompass stabilization, vitrification, soil washing, and electrokinetic processes. Meanwhile, bioremediation employs the inherent sequestration abilities of organisms like plants, bacteria, fungi, and algae. It's noteworthy that bioremediation stands out as an environmentally-friendly and cost-effective approach, crucial to the well-being of ecosystems. In cases of lead-contaminated water, widely adopted remedies encompass precipitation, coagulation-flocculation processes, ion interchange, adsorptive methods, and strategies rooted in membrane partitioning.

Given the advancements in lead management technologies and the sophistication of industrial decontamination techniques, it's anticipated that once the lead contamination issue is overcome, PSC will emerge as a potent source of pristine and sustainable energy.

4. Conclusion

At present, the main challenge faced by PSC is to achieve long-term stability at the component level and ensure long-term outdoor operation. Although the degradation of perovskite absorbents caused by moisture or oxygen in the ambient air can be inhibited by appropriate packaging, the performance degradation caused by light and heat should be solved by constructing stable materials and interfaces. The potential ecotoxicity caused by Pb is still hotly debated when considering the calcium titanium deposit. Drawing from the aforementioned findings, several potential mitigation tactics can be discerned to diminish the possible threats of PSC. One such approach includes the implementation of a consistent element addition method to enhance device efficiency, which in turn would govern the hazards and augment PCE. Notably, the toxicity of PSC towards humans and the environment may impede its commercial use. This concern transcends mere scientific boundaries, encompassing intricate legal and political dimensions. Consequently, scholars ought to aim not merely for heightened efficiency or absence of toxicity but also endeavor to strike a harmonious equilibrium between the two, maintaining them within permissible boundaries.

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