Report on Perovskite solar cells

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Abstract

Perovskite solar cells, based on organometal halide light absorbers, represent a revolutionary photovoltaic technology with the potential to transform the renewable energy landscape. Stemming from dye-sensitized solar cells, the journey of perovskite solar cells has been marked by rapid advancements. The technology's inception in liquid-based dye-sensitized solar cells yielded a modest power conversion efficiency (PCE) of around 3-4% in 2009. However, the liquid-based approach faced stability challenges due to the instant dissolution of perovskite in the electrolyte.

The transition to solid-state perovskite solar cells in 2012 marked a turning point, resulting in long-term stability and achieving PCE values of around 10%. In the years that followed, PCEs surged to 18% due to materials innovation and device design improvements. With the promise of PCE values surpassing 20%, perovskite solar cells have emerged as a compelling photovoltaic technology.

This thesis explores the opto-electronic properties of perovskite materials, recent breakthroughs in perovskite solar cell development, and the underlying challenges that need to be addressed for the technology's continued growth. While high efficiency and low material costs make perovskite solar cells attractive, stability issues remain a hurdle to commercialization. The review underscores the importance of holistic device design, intrinsic stability enhancements, and durable encapsulation materials to ensure the long-term viability of perovskite solar cells. Additionally, it delves into next-generation strategies aimed at pushing the power conversion efficiency beyond the Shockley-Queisser limit. The trajectory of perovskite solar cells, from their origins to their present state and future prospects, unfolds in this comprehensive exploration.

Introduction

The field of solar energy research has witnessed a paradigm shift in recent years with the emergence of Perovskite Solar Cells (PSCs) as a promising candidate for clean and sustainable energy generation. Perovskite materials, originally named after the Russian mineralogist L.A. Perovski, have garnered significant attention due to their unique crystal structure and exceptional electrical properties. These materials are characterized by the ABX3 formula, with X representing oxygen or a halogen, and are capable of exhibiting ferroelectricity or superconductivity.

Perovskite Solar Cells, with their distinctive properties and versatility, have the potential to revolutionize the renewable energy landscape. While the initial focus of perovskite research was on oxide-based materials, the introduction of organic-inorganic halide perovskites, such as CH3NH3PbX3 (X = Br, I), marked a significant turning point. These materials displayed a semiconductor-to-metal transition as their dimensionality increased, making them particularly attractive for solar cell applications. Researchers like Miyasaka and Park paved the way for this technology, achieving noteworthy power conversion efficiencies (PCE) with 3D perovskite materials.

Despite the early promise, challenges persisted, primarily related to the stability of organic-lead halide perovskites in liquid electrolytes. The breakthrough came with the development of solid-state perovskite solar cells, providing not only improved stability but also PCEs exceeding 9.7%. This pivotal achievement marked the dawn of a new era in solar cell technology.

Furthermore, research in this field extended to organic-inorganic layered perovskites, which have shown the potential to transition from insulators to metals by increasing the number of inorganic layers. Although initially overlooked due to lower photovoltaic performance and instability in liquid electrolytes, advancements in stability and efficiency led to a resurgence of interest in these materials. Recent developments have pushed PCEs to new heights, with the introduction of improved material compositions and deposition methods.

In this context, this thesis explores the remarkable journey of Perovskite Solar Cells, from their early discovery to the current state of the art. It delves into the materials, structures, and interface engineering techniques that have contributed to the advancement of PSCs. By understanding the device physics, the optoelectronic properties of perovskite materials, and the optimal fabrication processes, this research aims to shed light on the challenges and opportunities in this exciting field. With Perovskite Solar Cells being hailed as one of the most significant scientific breakthroughs, it is essential to comprehensively examine their past, present, and future.

Perovskite Materials

Perovskite materials have emerged as a game-changer in the field of solar energy and beyond. These versatile compounds, with their unique crystal structures and exceptional electronic properties, hold the promise of revolutionizing various technological applications. In this overview, we will delve into the world of perovskite materials, exploring essential subtopics that shed light on their significance.

Understanding Perovskite Structures:

At the heart of perovskite materials lies their intriguing crystal structure. Understanding this structure is fundamental to unlocking their potential. Perovskites adhere to the ABX3 formula, with the A-site occupied by a larger cation, the B-site by a smaller cation, and X representing anions, usually oxygen or a halogen. This section unravels the intricacies of perovskite structures, including their cubic, tetragonal, and orthorhombic phases, and the impact of structural variations on their properties.

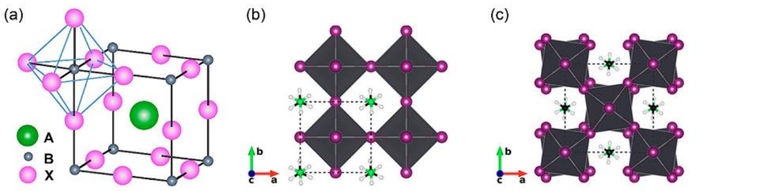


Figure 7. (a) Perovskite crystal structure. For photovoltaically interesting perovskites, the large cation (A) is usually the methylammonium ion (CH_3NH_3), the small cation (B) is Pb, and the X anion is a halogen ion (usually I, although both Cl and Br are also receiving attention). For $CH_3NH_3PbI_3$, the cubic phase forms only at temperatures above 330 K. Reproduced with permission from ref 48. Copyright 2015 Elsevier. Schematic structural representation of $MAPbI_3$, where MA = methylammonium in the (b) pseudocubic and (c) tetragonal phases. The thick dashed lines indicate the unit cell, which contains C (black), N (green), H (white), I (violet), and Pb (light gray) atoms; the highest symmetry phase for $MAPbI_3$ and its related materials is the cubic ($Pm\bar{3}m$) lattice phase, with sequential transitions lowering the symmetry typically through octahedral tilting. The tilting collectively leads to the transition from the cubic to tetragonal phase. Reproduced with permission from ref 50. Copyright 2013 American Chemical Society.

Key Materials Used in Perovskite Solar Cells:

Perovskite solar cells have garnered significant attention for their remarkable efficiency and low-cost fabrication. This subtopic delves into the key materials employed in perovskite solar cells. We'll explore the role of organic-inorganic hybrid perovskites, such as methylammonium lead iodide (CH3NH3PbI3), and their all-inorganic counterparts in achieving high photovoltaic performance.

Crystallography and Electronic Properties:

Crystallography and electronic properties are at the heart of perovskite materials' remarkable characteristics. We will take a closer look at the crystallographic aspects of perovskites, including their lattice structures and the influence of temperature on phase transitions. Additionally, we'll delve into the electronic properties, highlighting the bandgap, carrier mobility, and electronic structure that make perovskites ideal for photovoltaic applications.

Hybrid Organic-Inorganic Perovskites vs. All-Inorganic Perovskites:

The choice between hybrid organic-inorganic perovskites and all-inorganic perovskites is a critical consideration in perovskite material research. This section explores the advantages and disadvantages of each type. Hybrid perovskites, like CH3NH3PbI3, offer tunable bandgaps and excellent optoelectronic properties. On the other hand, all-inorganic perovskites, such as CsPbI3, are known for their enhanced stability and potential in tandem solar cell configurations.

Device Architectures

Common device architectures

The two most common device architectures for solar cells are the n-i-p and p-i-n configurations. In the n-i-p configuration, the light-absorbing layer is sandwiched between an electron transport layer (ETL) and a hole transport layer (HTL). The ETL collects the electrons generated in the light-absorbing layer and transports them to the electrode. The HTL collects the holes generated in the light-absorbing layer and transports them to the other electrode.

In the p-i-n configuration, the light-absorbing layer is sandwiched between a hole transport layer (HTL) and an electron transport layer (ETL). The HTL collects the holes generated in the light-absorbing layer and transports them to the electrode. The ETL collects the electrons generated in the light-absorbing layer and transports them to the other electrode.

Electron and Hole Transport Layers

The electron and hole transport layers play an important role in the performance and stability of solar cells. The ETL must have a high electron mobility and a low bandgap to efficiently collect and transport electrons. The HTL must have a high hole mobility and a high bandgap to efficiently collect and transport holes.

Common ETL materials include:

- Titanium dioxide (TiO2)
- Zinc oxide (ZnO)
- Tin oxide (SnO2)
- Phenyl-C61-butyric acid methyl ester (PCBM)

Common HTL materials include:

- Spiro-OMeTAD
- Poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS)
- Poly[N,N'-bis(4-butylphenyl)-1,1-biphenyl-4,4'-diamine] (PBD)

Interface Engineering for Improved Efficiency

The interfaces between the different layers in a solar cell play an important role in the device performance. Poor interfaces can lead to charge recombination, which reduces the efficiency of the solar cell.
Interface engineering is a technique used to improve the quality of the interfaces in a solar cell. This can be done by using thin interfacial layers, doping the layers, or using surface modification techniques.
For example, a thin layer of lithium fluoride (LiF) can be used to improve the interface between the perovskite light-absorbing layer and the electron transport layer in perovskite solar cells. This is because LiF has a high electron mobility and a low bandgap, which helps to reduce charge recombination at the interface.

Stability and Encapsulation Considerations

Solar cells need to be stable in order to have a long lifetime. This means that they need to be able to withstand environmental factors such as moisture, oxygen, and UV light.
Encapsulation is a technique used to protect solar cells from the environment. This can be done by coating the solar cell with a thin layer of material, such as glass or plastic.
Encapsulation is especially important for perovskite solar cells, which are more sensitive to the environment than other types of solar cells.

Emerging Device Architectures

In addition to the traditional n-i-p and p-i-n configurations, there are a number of emerging device architectures that are being developed for solar cells. These include:

- Tandem solar cells: Tandem solar cells use two or more light-absorbing layers with different bandgaps to absorb a wider range of the solar spectrum. This can lead to higher efficiency solar cells.
- Perovskite-based solar cells: Perovskite solar cells are a new type of solar cell that has achieved very high efficiencies in a short period of time. Perovskite solar cells are still under development, but they have the potential to become a leading solar cell technology in the future.

Performance and Efficiency

Record Efficiency Achievements in Perovskite Solar Cells:

Perovskite solar cells have achieved remarkable progress in recent years, with rapid increases in efficiency. The current world record efficiency for a single-junction perovskite solar cell is 25.7%, and the record efficiency for a tandem perovskite-silicon solar cell is 29.8%. These efficiencies are comparable to those of commercial silicon solar cells and, in some cases, even exceed them. This suggests that perovskite solar cells have the potential to become a leading solar cell technology in the future.

Factors Influencing Efficiency Improvements:

Several key factors have contributed to the recent improvements in perovskite solar cell efficiency:

- Improved Understanding of Perovskite Materials: Researchers have gained a better understanding of the fundamental properties of perovskite materials, which has led to the development of new and improved perovskite compositions.

- Better Device Fabrication Techniques: Device fabrication techniques have improved significantly in recent years, leading to more uniform and higher-quality perovskite films.
- Development of New Materials for Electron and Hole Transport Layers: New materials have been developed for the electron and hole transport layers in perovskite solar cells, which have led to improved charge collection and transport.
- Interface Engineering: Researchers have developed new interface engineering techniques to reduce charge recombination at the interfaces between the different layers in a perovskite solar cell.

Stability and Hysteresis Challenges:

One of the main challenges facing perovskite solar cells is stability. Perovskite materials are sensitive to moisture and oxygen, which can degrade the device performance and lifetime. Additionally, hysteresis, a phenomenon where the current-voltage curve of a perovskite solar cell depends on the scan direction, can lead to inaccurate efficiency measurements and reduce the performance of perovskite solar cells under real-world operating conditions.

Strategies to Enhance Efficiency and Stability:

- Researchers are actively pursuing various strategies to enhance the efficiency and stability of perovskite solar cells:
- Developing New Perovskite Materials with Improved Stability: Researchers are working on new perovskite materials that are more resistant to moisture, oxygen, and UV light.
- Using Encapsulation Techniques: Encapsulation techniques, such as coating the solar cell with a thin layer of glass or plastic, can protect the perovskite layer from environmental factors, enhancing stability.
- Developing Stable Electron and Hole Transport Layers: New electron and hole transport layers that are more stable can improve the overall stability of perovskite solar cell devices.
- Interface Engineering for Reduced Hysteresis: Interface engineering techniques are being employed to enhance the quality of interfaces between different layers in perovskite solar cells, reducing hysteresis and improving both efficiency and stability.

Key Challenges in Achieving High Efficiency

1. Structure Design:

- Crystal Structure: The crystal structure of perovskite materials is crucial in determining their electronic and optoelectronic properties. Achieving a stable and well-defined crystal structure, typically a simple cubic lattice, is essential. Phase transitions, such as from cubic to tetragonal or orthorhombic, can significantly impact the material's behaviour. Understanding and controlling these structural transitions is key to optimizing perovskite performance.
- Defect Structure: Minimizing defects within the perovskite structure is vital for enhancing efficiency. Defects, like vacancies and impurities, can trap and recombine charge carriers, reducing overall performance. Researchers focus on characterizing and mitigating these defects to create high-quality perovskite materials.
- Microstructure: The microstructure of perovskite films plays a critical role in determining how efficiently charge carriers can move through the material. Engineering the microstructure can lead to improved charge carrier transport and reduced hysteresis, which is a challenge in perovskite solar cells, where the current-voltage curve depends on the scan direction.

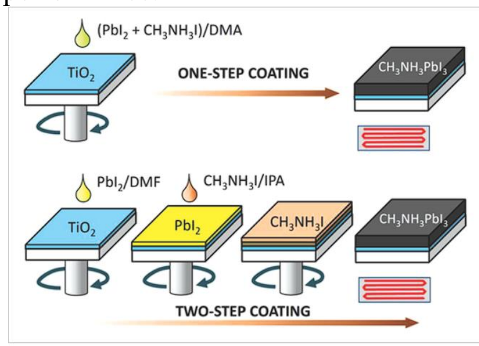
2. Materials Chemistry:

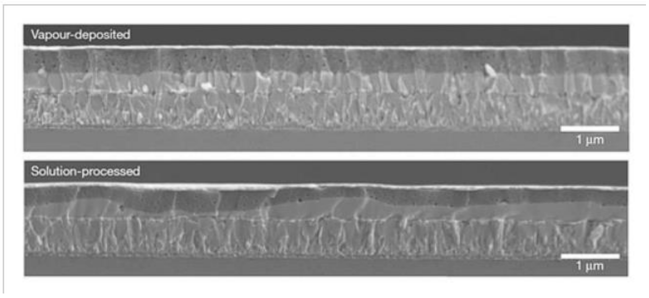
- A Site (Cation)-Modified Perovskites: Modifying the A-site cations in perovskite structures involves replacing the large methylammonium (MA) ions with other species. This can enhance stability, bandgap tuning, and optoelectronic properties. Exploring different A-site cations is essential to tailor perovskite materials for specific applications.

- B Site (Cation)-Modified Perovskites: Tailoring the B-site cations involves changing the central metal ions (e.g., Pb) in the perovskite structure. This modification can optimize charge transport and reduce defects within the material, leading to enhanced device performance.
- X Site (Anion)-Modified Perovskites: Substituting anions (usually I, Cl, or Br) in the X site allows researchers to fine-tune properties like bandgap and stability. Understanding the effects of anion substitution is vital for designing perovskites with improved performance characteristics.
- Low-Dimensional Perovskites: Low-dimensional perovskites, such as quantum wells or superlattices, offer advantages in terms of carrier transport and stability. By exploring these alternative structures, researchers aim to achieve more efficient and stable perovskite solar cells.

3. Processing Engineering:

- One-Step vs. Two-Step Processes: Fabrication processes are critical for creating high-quality perovskite films. One-step and two-step methods are commonly used. Researchers focus on optimizing these processes to control film morphology and minimize defects, ultimately leading to improved device performance.





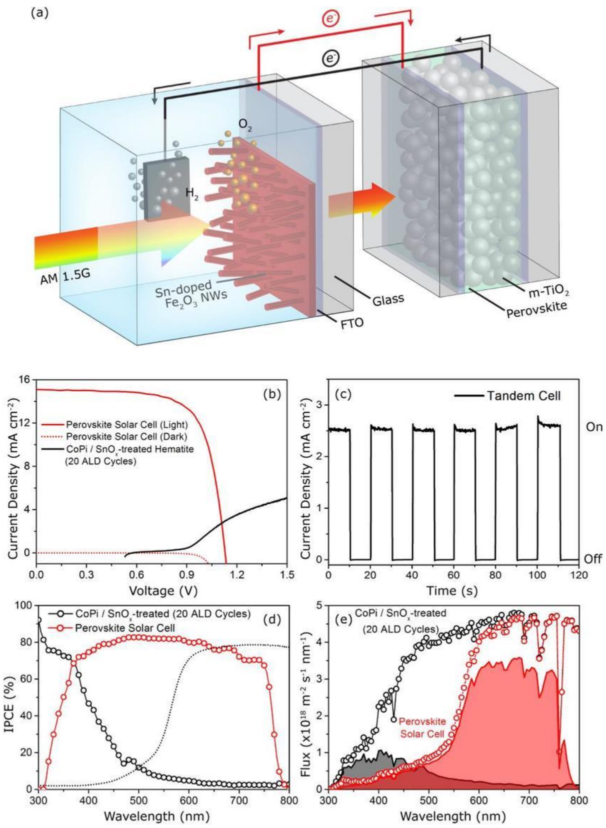
- Adduct Intermediated Process: Innovative techniques like adduct formation are explored to enhance perovskite film formation. These methods offer precise control over film quality, grain size, and defect density, resulting in solar cells with improved efficiency and stability.

4. Device Physics:

- Selective Contact: Achieving efficient selective contacts is essential for extracting charge carriers while minimizing energy losses during transport. The design of contacts that can efficiently match energy levels with perovskite materials is a key challenge.
- Interface Engineering: Interfaces between different layers within a perovskite solar cell are critical. Researchers work on optimizing these interfaces to reduce charge recombination, improve charge extraction, and enhance device performance.
- Defect Passivation: Identifying and mitigating defects within the perovskite material is crucial for achieving high efficiency. Various passivation techniques are investigated to improve charge carrier lifetime and reduce recombination rates.

5. Over Shockley–Queisser Limit:

- Tandem Solar Cells: Tandem solar cell architectures involve stacking multiple photovoltaic layers to capture excess energy beyond the Shockley-Queisser limit. Developing efficient tandem designs is a complex challenge, but it holds the potential to significantly increase solar cell efficiency.



- Hot Carrier Devices: Hot carrier devices aim to capture and utilize high-energy carriers, reducing energy losses and increasing efficiency. This approach requires careful engineering to harness the benefits of hot carriers effectively.

Reference:

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