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REVIEW

Artificial intelligence in Perovskite-Based materials for energy applications

Inteligencia artificial en materiales basados en Perovskita para aplicaciones energéticas

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ABSTRACT

Introduction: Perovskite-based materials have gained significant attention in energy applications due to their remarkable optoelectronic properties and versatile composition. These materials, characterized by their ABX_3 crystal structure, have demonstrated high efficiencies in solar cells, light-emitting diodes (LEDs), and potential in energy storage systems.
Objective: Perovskite solar cells (PSCs) have achieved efficiencies comparable to silicon-based cells, with advantages in cost and fabrication flexibility.
Method: a literature review was conducted, including original articles, reviews, and bibliometric studies. The research focused on AI in Perovskite-Based Materials for Energy Applications.
Result: AI is driving significant advancements in the field of perovskite-based materials for energy applications.
Conclusion: Perovskite LEDs offer high color purity and tunable emission, making them ideal for display technologies. Despite challenges like stability and scalability, ongoing research aims to enhance their performance, positioning perovskites as key materials in sustainable energy technologies. By accelerating material discovery, optimizing manufacturing processes, enhancing stability and performance, and promoting sustainability.

Keywords: Artificial Intelligence; Perovskite LEDs; Energy; Solar Cells.

RESUMEN

Introducción: los materiales basados en perovskita han ganado una atención significativa en aplicaciones energéticas debido a sus notables propiedades optoelectrónicas y composición versátil. Estos materiales, caracterizados por su estructura cristalina ABX_3, han demostrado altas eficiencias en células solares, diodos emisores de luz (LED) y potencial en sistemas de almacenamiento de energía.
Objetivo: las células solares de perovskita (PSC) han alcanzado eficiencias comparables a las células basadas en silicio, con ventajas en coste y flexibilidad de fabricación.
Método: se realizó una revisión bibliográfica que incluyó artículos originales, revisiones y estudios bibliométricos. La investigación se centró en la IA de los materiales basados en la perovskita para aplicaciones energéticas.
Resultados: la IA está impulsando avances significativos en el campo de los materiales basados en la perovskita para aplicaciones energéticas.
Conclusiones: los LED de perovskita ofrecen una gran pureza de color y una emisión sintonizable, lo que los

hace ideales para las tecnologías de visualización. A pesar de problemas como la estabilidad y la escalabilidad, las investigaciones en curso pretenden mejorar su rendimiento, situando a las perovskitas como materiales clave en las tecnologías energéticas sostenibles. Acelerando el descubrimiento de materiales, optimizando los procesos de fabricación, mejorando la estabilidad y el rendimiento y fomentando la sostenibilidad.

Palabras clave: Inteligencia Artificial; Leds De Perovskita; Energía; Células Solares.

INTRODUCTION

Perovskite-based materials have revolutionized the field of energy applications due to their unique structural properties, exceptional optoelectronic characteristics, and relatively low-cost fabrication methods. Characterized by the general formula ABX_3, where 'A' is a large cation, 'B' is a smaller metal cation, and 'X' is an anion such as a halide, perovskites exhibit a versatile crystal structure that can be tailored for a wide range of applications, including solar cells, light-emitting diodes (LEDs), photodetectors, and energy storage devices. This adaptability has positioned perovskites as frontrunners in the quest for high-efficiency, cost-effective energy solutions.

The most notable success of perovskite materials is in the field of photovoltaics, where perovskite solar cells (PSCs) have achieved rapid advancements in power conversion efficiencies, surpassing 25 % within a decade of development. This remarkable progress is largely attributed to the superior light absorption, tunable bandgap, and excellent charge-carrier mobility of perovskites, which allow them to compete with traditional silicon-based solar technologies. Additionally, the ability to process perovskites at low temperatures using solution-based methods offers a significant reduction in manufacturing costs, opening pathways for the development of lightweight, flexible, and semi-transparent solar cells that can be integrated into a variety of surfaces. Beyond photovoltaics, perovskite materials are making significant inroads in other energy applications. Perovskite LEDs (PeLEDs) have shown great promise for next-generation display and lighting technologies due to their high color purity, tunable emission, and efficient light emission properties. Furthermore, the potential of perovskites extends to energy storage, where their unique ionic conductivity and redox properties make them suitable candidates for use in batteries and supercapacitors. These diverse applications highlight the versatility and broad appeal of perovskite materials in the energy sector. Despite their numerous advantages, perovskite-based materials face several challenges that must be addressed before they can achieve widespread commercial adoption. Stability remains a critical issue, as many perovskite compounds are susceptible to degradation when exposed to moisture, heat, and UV light. Additionally, the presence of lead in many high-performance perovskites raises environmental and health concerns, prompting the need for lead-free alternatives that do not compromise efficiency. Addressing these challenges through materials engineering, advanced device architectures, and innovative fabrication techniques is essential for the continued advancement of perovskite-based technologies.

This paper aims to explore the current state of perovskite-based materials for energy applications, with a focus on recent advancements, ongoing challenges, and future prospects. By examining the latest research and development efforts, this review seeks to provide a comprehensive overview of how perovskites are shaping the future of sustainable energy technologies.

Literature Review

Perovskite-based materials have garnered significant interest in energy applications due to their exceptional optoelectronic properties, cost-effectiveness, and versatility in composition. This review explores the latest research contributions from ten different studies, highlighting advancements in perovskite solar cells (PSCs), light-emitting diodes (LEDs), and energy storage devices.

Advancements in Perovskite Solar Cells

Recent work investigated the stability of perovskite solar cells by introducing a double-layered encapsulation approach, which significantly improved device longevity under ambient conditions. Their study showed that the encapsulated PSCs maintained 90 % of their initial efficiency after 1,000 hours of continuous illumination, demonstrating progress towards commercial viability.[(1)] Similarly, an study developed a novel mixed-cation perovskite formulation that enhanced both efficiency and stability.[(2)] By incorporating rubidium and cesium into the perovskite structure, they achieved a power conversion efficiency of 26,1 %, with excellent thermal and moisture stability, paving the way for next-generation high-performance PSCs.

Perovskite LEDs and Display Technologies

In the field of light-emitting diodes, focused on improving the color purity and operational stability of

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perovskite LEDs, by employing a core-shell nanoparticle approach, their LEDs exhibited narrow emission peaks and a significant increase in operational lifetime, making them suitable for high-definition display applications.[3] Meanwhile, other article explored the use of perovskites in flexible LEDs, highlighting the potential for wearable and foldable electronic devices. Their research demonstrated that flexible PeLEDs could maintain high performance even under mechanical stress, suggesting robust application in next-generation electronic displays.[4]

Hybrid Perovskite Structures for Enhanced Performance

An study introduced a hybrid perovskite structure by integrating 2D perovskites with 3D counterparts, resulting in improved charge transport and reduced non-radiative losses. This hybrid approach led to enhanced device performance, with significant implications for both solar cells and LEDs. Similarly, other research explored 2D/3D perovskite heterojunctions for energy storage applications, particularly in supercapacitors. Their study found that the hybrid perovskite structures offered higher capacitance and better cycling stability compared to conventional electrode materials, opening new avenues for perovskite-based energy storage solutions.

Energy Storage and Catalysis

In the realm of energy storage, a research examined the use of perovskites as cathode materials in lithium-ion batteries. Their research demonstrated that doping perovskites with transition metals such as manganese and cobalt improved the electrochemical performance, resulting in higher capacity retention and longer battery life.[5] Furthermore, Zhao et al. (2022) investigated perovskites in catalysis for hydrogen evolution reactions (HER). By optimizing the surface chemistry of perovskites with catalytic additives, they achieved enhanced hydrogen production rates, highlighting the potential of perovskites in clean energy technologies.[6]

Scalability and Environmental Impact

Addressing the challenges of scalability, Patel et al. (2023) developed a roll-to-roll printing technique for the mass production of perovskite solar modules. Their work demonstrated that large-area PSCs could be fabricated with minimal loss of efficiency, representing a critical step towards commercial-scale deployment.[7] To tackle the environmental concerns associated with lead-based perovskites, Smith et al. (2023) explored lead-free alternatives using tin-based perovskites. Although these alternatives currently lag behind in efficiency, their research highlighted promising pathways for reducing toxicity while maintaining reasonable performance, supporting the development of more sustainable perovskite materials.[8]

Perovskite Solar Cells (PSCs)

Perovskite solar cells have gained substantial attention due to their remarkable efficiency improvements over a relatively short period. Since the first reported efficiency of 3,8 % in 2009, PSCs have achieved efficiencies exceeding 25 %, rivaling those of conventional silicon-based solar cells. The rapid progress in efficiency is largely attributed to the tunability of perovskite materials, which allows for the optimization of their bandgap, stability, and charge transport properties. One of the primary advantages of PSCs is their ability to absorb a broad range of the solar spectrum, including visible and near-infrared light. This wide absorption range, combined with high photoluminescence quantum yields, makes perovskites highly efficient at converting sunlight into electricity. Moreover, the thin-film nature of perovskites enables the production of lightweight and flexible solar cells, which can be integrated into a variety of surfaces, including building facades, windows, and even wearable devices.

Despite these advantages, PSCs face several challenges that must be addressed to achieve commercial viability. The most significant issue is their long-term stability, as perovskite materials are prone to degradation when exposed to moisture, oxygen, and heat. Research efforts are currently focused on enhancing the stability of perovskite layers through compositional engineering, the incorporation of protective coatings, and the development of robust encapsulation techniques.

Perovskite Light-Emitting Diodes (LEDs)

In addition to their application in solar cells, perovskite materials have shown great potential in light-emitting diodes (LEDs). Perovskite LEDs (PeLEDs) leverage the excellent luminescent properties of perovskites, including high color purity, tunable emission wavelengths, and high quantum efficiencies. These properties are particularly advantageous for display technologies, where vivid and accurate color reproduction is essential.[9]

PeLEDs can be fabricated using solution processing, which is not only cost-effective but also allows for the production of large-area and flexible devices. The ability to fine-tune the emission wavelength of perovskites by adjusting their composition further enhances their appeal for next-generation display and lighting applications. However, similar to PSCs, the stability of PeLEDs remains a concern. Efforts to improve device stability include the use of more stable perovskite compositions, as well as advanced device architectures that protect the

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perovskite layer from environmental degradation.

Perovskite Materials in Energy Storage

Beyond photovoltaic and lighting applications, perovskite materials are also being explored for energy storage, particularly in lithium-ion batteries and supercapacitors. The high ionic conductivity and tunable redox properties of perovskites make them suitable candidates for electrode materials in batteries. In supercapacitors, perovskites can contribute to high capacitance and energy density due to their ability to store and release charge rapidly.[8]

The use of perovskites in energy storage devices is still in its early stages, with ongoing research aimed at optimizing their electrochemical performance and cycling stability. Innovations in this area could lead to more efficient and sustainable energy storage solutions, complementing the role of perovskites in renewable energy generation.

Role of AI in Perovskite-Based Materials for Energy Applications

Artificial Intelligence (AI) is playing an increasingly pivotal role in the advancement of perovskite-based materials for energy applications. The rapid evolution of AI techniques, particularly in machine learning (ML) and data-driven modeling, has provided powerful tools for accelerating the discovery, optimization, and deployment of perovskite materials. AI's ability to handle vast datasets, identify complex patterns, and predict material properties with high accuracy is transforming how researchers approach the challenges in developing perovskite-based energy solutions such as solar cells, LEDs, and energy storage devices.[10]

Accelerated Materials Discovery and Optimization

AI and ML algorithms are revolutionizing the materials discovery process by significantly reducing the time and resources required to identify new perovskite compositions with desired properties. Traditional methods of material synthesis and characterization are often time-consuming and expensive. AI-driven techniques, such as high-throughput virtual screening and predictive modeling, enable researchers to explore vast chemical spaces and predict the performance of novel perovskite compounds before experimental validation. For example, using ML models trained on existing datasets, researchers can predict key material properties like bandgap, stability, and charge-carrier mobility, guiding the synthesis of new perovskites with optimized characteristics for specific energy applications.[11]

A notable application of AI in this domain is the use of neural networks and genetic algorithms to predict and optimize the composition of perovskite materials for enhanced solar cell performance. These models can identify optimal combinations of elements and processing conditions that maximize efficiency while maintaining stability. Such approaches have already led to the discovery of new perovskite formulations with improved tolerance to environmental factors, addressing one of the key challenges in the commercialization of perovskite solar cells.

Improving Device Stability and Performance

Stability remains a major hurdle for perovskite-based materials, particularly in the context of solar cells and LEDs. AI techniques are being applied to tackle this challenge by modeling degradation mechanisms and predicting the long-term performance of perovskite devices under various environmental conditions. By analyzing data from accelerated aging tests, ML models can identify factors that contribute to material degradation, such as moisture, heat, and UV exposure. This knowledge enables the design of more robust perovskite formulations and protective coatings that enhance device longevity.

In addition, AI-driven optimization can improve the performance of perovskite devices by fine-tuning the interface engineering between perovskite layers and other components in the device stack. For example, reinforcement learning algorithms can be used to explore a wide range of interface materials and configurations, ultimately leading to improved charge transport and reduced recombination losses in solar cells and LEDs.

Enhanced Predictive Maintenance and Performance Monitoring

AI also plays a crucial role in the operational phase of perovskite-based energy devices. Predictive maintenance models, powered by machine learning, can monitor the performance of deployed perovskite solar panels or LEDs, predicting potential failures before they occur. These models analyze data from sensors embedded in the devices to track performance metrics, detect anomalies, and forecast maintenance needs, thereby extending the operational lifespan of the devices and reducing downtime.

Challenges and Future Prospects

While perovskite-based materials offer numerous advantages, several challenges must be addressed to realize their full potential in energy applications. Stability remains a critical issue across all perovskite-based devices,

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with ongoing research dedicated to improving the durability of these materials under operational conditions. Additionally, concerns related to the environmental impact of lead-containing perovskites have prompted the search for alternative, less toxic materials without compromising performance. Another area of focus is the scalability of perovskite production. While laboratory-scale devices have demonstrated impressive results, scaling up the manufacturing processes while maintaining efficiency and stability is a complex challenge. Efforts are underway to develop scalable fabrication techniques, such as roll-to-roll printing and vapor deposition, which could facilitate the commercialization of perovskite technologies.

Looking ahead, the integration of perovskites with other materials and technologies presents exciting opportunities for innovation. Tandem solar cells, which combine perovskites with silicon or other materials, have shown potential for achieving even higher efficiencies than single-junction cells. Additionally, hybrid devices that incorporate perovskites in conjunction with other energy conversion and storage technologies could lead to multifunctional energy systems that optimize both generation and storage.

CONCLUSIONS

Perovskite-based materials represent a transformative development in the field of energy applications, offering significant advantages in terms of efficiency, cost, and versatility. Their unique optoelectronic properties and ease of fabrication make them highly attractive for a range of technologies, including solar cells, LEDs, and energy storage devices. While challenges related to stability, scalability, and environmental impact remain, ongoing research and innovation continue to drive progress in this rapidly evolving field. With continued advancements, perovskite-based materials have the potential to play a crucial role in the global transition to sustainable energy, contributing to a future of clean and efficient energy solutions. conclusion, AI is driving significant advancements in the field of perovskite-based materials for energy applications. By accelerating material discovery, optimizing manufacturing processes, enhancing stability and performance, and promoting sustainability, AI is unlocking the full potential of perovskites as next-generation energy solutions. As AI techniques continue to evolve, their integration into the research and development of perovskite materials will play a critical role in overcoming existing challenges and scaling these technologies for widespread use in a sustainable energy future.

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