

Key Applications and Frontier Breakthroughs of Nanomaterials in the Next Generation of Photovoltaic Technology

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Abstract. This article reviews the current research status and advancements of nanomaterials in the field of next-generation photovoltaic technology. It begins by highlighting the key applications and significance of nanomaterials in this field, emphasizing their practical importance. The article then systematically summarizes the cutting-edge breakthroughs of these materials in photovoltaic technology. By analyzing relevant literature from both domestic and international sources, it provides a detailed overview of the main achievements and progress in photovoltaic technology research abroad, as well as an introduction to the current research status and characteristics in China. Through a comparison of domestic and international research, the article identifies several hot topics and challenges in the photovoltaic research field, particularly in terms of stability, large-scale production, and environmentally friendly materials. Finally, the article offers a comprehensive review of existing research, highlights the current research challenges, and suggests future research directions and potential trends. The aim is to provide a reference for researchers in the field of nano-photovoltaic materials and to offer some ideas and suggestions for future research.

Keywords: nanomaterials, photovoltaic technology, single atom catalyst

1. Introduction

In recent years, since the 21st century, in the context of serious energy crises and environmental pollution, carbon peak and carbon neutrality [1]. Under the policy guidance, China urgently needs to develop new technologies to meet the comprehensive needs of all aspects, so perovskite solar cells (PSCs) and quantum dots [2]. New photovoltaic technologies, including quantum dot solar cells (QDSCs), organic photovoltaics (OPV), and silicon-based tandem cells, have seen rapid development, setting new records in photovoltaic conversion efficiency. However, their commercialization is still hindered by issues such as poor stability, difficulties in large-scale production, and environmental toxicity. Particularly, the conflict between cost control and green manufacturing needs to be addressed urgently. Current research in advanced technologies primarily focuses on metamaterials and super-surfaces, interface modification of single-atom-layer materials, dynamic defect repair of self-healing nanomaterials, and flexible and transparent photovoltaic technologies. This study focuses on innovative applications of nanomaterials in the photovoltaic

field. By summarizing literature, it explores the balance between cutting-edge technology and practical production. This research not only provides theoretical support for optimizing stability and efficiency in tandem cells but also lays the groundwork for photovoltaic technology to evolve towards low cost, high stability, and environmental friendliness, which is crucial for advancing the industrialization of clean energy technologies.

Metamaterials [3] are a new type of optical material that overcomes the physical limitations of natural materials through the design of artificial micro-nano structures. These metamaterials consist of three-dimensional sub-wavelength units, enabling negative refraction and electromagnetic stealth. In contrast, metasurfaces are two-dimensional planar structures that precisely control the phase, amplitude, and polarization of light through nano-structure arrays, offering advantages such as ultra-thinness and low loss. In the field of light management, their applications include replacing traditional optical components with planar lenses, controlling beam deflection and focusing, holographic imaging, and spectral analysis, significantly enhancing light utilization and promoting device miniaturization. When combined with phase change materials, these properties are further enhanced [4]. For example, GeSbTe dynamic hypersurfaces can achieve beam switching, tunable holography, and other functions, and can be integrated with LED, photovoltaic and other systems to optimize energy efficiency.

It is worth noting that Tao Guangming from Huazhong University of Science and Technology, along with Yang Haochuan from Zhejiang University and other scholars, has achieved efficient preparation of polymer functional microspheres using the fiber core laminar flow mechanics method (PRI method), as shown in Figure 1. This method leverages the instability of the fluid interface within the fibers, utilizing the Plateau-Rayleigh effect to induce the destabilization and rupture of the core layer fluid through thermal stretching of the fibers. It can precisely control the particle size of the microspheres (ranging from 20 nm to 1.25 μm), overcoming the limitations of traditional solution methods. The method offers advantages such as single dispersion, cost control, and high yield. These microspheres find extensive applications in medicine (such as clinical diagnosis and drug delivery), sensing, and optics. They can be functionalized by doping with magnetic nanoparticles, quantum dots, or biomolecules, for example, to achieve functions like magnetic adsorption of heavy metals, fluorescence detection, and targeted biosensing. Additionally, they can be designed into preform structures to create complex microspheres with core-shell or Janus structures. In recent years, the use of CO₂ laser local heating and 3D printing technology has further optimized the uniformity of particle size and the flexibility of structural design, providing a new approach for the development of multifunctional integrated microspheres [5].

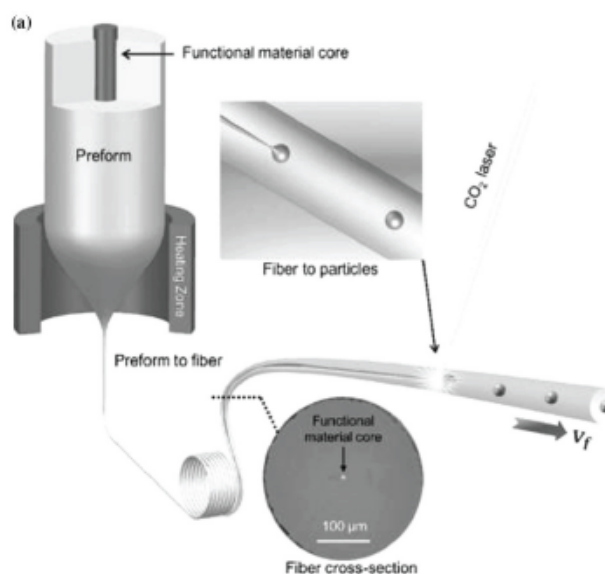


Figure 1: Schematic diagram of multi-material fiber stretching and carbon dioxide laser assisted fiber particle preparation [5]

Nanomaterials face three major challenges in their application and promotion: stability, large-scale production, and environmental friendliness. In terms of stability, their high surface energy can lead to agglomeration or chemical degradation, which requires surface modification and structural optimization to enhance corrosion resistance and dispersion. Large-scale production is hindered by difficulties in scaling up processes and high costs, necessitating the use of green synthesis technologies, automated control, and continuous production to achieve efficient preparation. Environmental friendliness involves addressing potential toxicity and pollution issues, which can be mitigated through clean processes, biocompatible design, and closed-loop recycling to reduce ecological risks. Future efforts should integrate interdisciplinary innovation and policy guidance to promote sustainable development in areas such as energy and healthcare.

2. Single atomic layer materials

Single atomic layer materials are two-dimensional materials composed of a single layer of atoms or molecules, with atomic thickness (0.1-0.3 nm), high specific surface area and quantum confinement effect [6]. It exhibits excellent electron mobility, uniform active sites, and flexible stability. In catalysis, its applications include electrocatalytic hydrogen evolution (such as the synergistic catalysis of ruthenium clusters with oxygen-coordinated iron monomers), CO₂ conversion (where two-dimensional iridium monolayers regulate reaction pathways), and non-noble metal catalysis (such as cobalt monomer degradation of organic pollutants). In terms of interface regulation, precise optimization of electronic structure and reaction activity can be achieved through heterostructure charge recombination (such as the transition from insulator to metal via iridium oxide superlattices), strong metal-support interactions (such as CNT-V-Fe anchored ruthenium clusters), and coordination environment design (such as porphyrin-based monomers regulating CO₂ reduction selectivity). These materials show great potential in energy conversion, environmental remediation, and quantum devices, such as room-temperature quantum anomalous Hall effect.

Scholars, including Shi Yantao from Dalian University of Technology, successfully prepared a honeycomb nitrogen-doped porous carbon-supported iron-based single-atom catalyst (Fe SA-NC)

using a molten salt-assisted pyrolysis method (Figure 2). This catalyst uses hypoxanthine as the carbon and nitrogen source, and the strong polarizing environment of ZnCl_2/KCl molten salt inhibits the high-temperature sintering of iron atoms, forming an Fe-N_4 coordination structure. The catalyst features a high specific surface area ($2072 \text{ m}^2\cdot\text{g}^{-1}$) and a rich pore structure. AC-HAADF-STEM and XAFS confirmed that the iron is dispersed in isolated single-atom form. In oxygen reduction reactions (ORR), Fe SA-NC exhibits excellent catalytic activity, with a half-wave potential of 0.85 V (0.1 M KOH) and a maximum current density of $5.79 \text{ mA}\cdot\text{cm}^{-2}$, surpassing commercial Pt/C catalysts. It also shows high selectivity for the four-electron pathway (H_2O_2 yield $<2\%$). Additionally, it demonstrates good resistance to methanol interference and long-term stability (no activity decay after 10,000 CV cycles). The pore formation, defect regulation, and atomic dispersion effects of the molten salt collectively enhance its performance. This study provides a new strategy for the low-cost, large-scale preparation of single-atom catalysts, with significant potential applications [7].

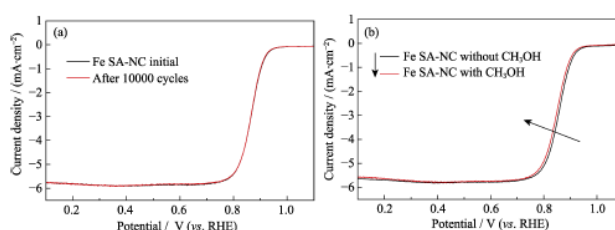


Figure 2: Durability test and methanol resistance test of Fe SA-NC in oxygen saturated 0.1 mol/L KOH solution at 1600 r/min (a) and (b)[7]

Single-atom-layer materials face three major challenges in their application and promotion: stability, large-scale production, and environmental friendliness. In terms of stability, the atomic-thickness material is highly sensitive to mechanical stress, thermal fluctuations, and chemical environments. The high activity sites at the edges can easily lead to performance degradation. To enhance durability, methods such as doping, heterostructure design, surface protection (coating encapsulation or substrate support), and edge passivation (chemical modification) are necessary. For large-scale production, traditional methods like mechanical exfoliation and CVD are limited by low efficiency, high costs, and transfer damage. Therefore, electrochemical exfoliation and biological methods need to be developed [8]. Direct in-situ growth (such as roll-to-roll CVD) and defect-controlled preparation; environmental friendliness requires solving pollution (strong acid/catalyst dependence) and resource consumption in the preparation process, which can be achieved through resource recycling (catalyst recovery) and life cycle management to achieve sustainable development [9]. In the future, interdisciplinary innovation and system optimization should be combined to promote the industrialization process.

3. Flexible and transparent photovoltaic

Flexible and transparent photovoltaics are two major development directions of new photovoltaic technology. The former uses organic materials and perovskite [10]. Thin-film technology enables lightweight and flexible devices, while the latter utilizes semi-transparent electrodes and bandgap modulation to balance power generation and light transmission. In recent years, advancements in material innovation (such as silver nanowire electrodes and biomimetic fractal structures) and structural optimization (such as dynamic stretching design and phase change transparency control) have significantly boosted efficiency. For instance, perovskite batteries can achieve a visible light

transmittance of over 40% by adjusting their thickness, and they are advancing towards industrialization through roll-to-roll printing technology. The applications have expanded from wearable devices to photovoltaic building integration (BIPV) [11]. In the future, it is necessary to break through the balance of efficiency, flexibility and cost, and is expected to become an important clean energy carrier under the carbon neutral target.

Zhou Yin-hua and colleagues from Huazhong University of Science and Technology conducted a study on the solvent damage to the lower hole transport layer (HTL) of poly (3,4-ethylenedioxythiophene): perfluorosulfonic acid ion polymer (PEDOT:F) during the coating process of silver nanowire (AgNWs) top electrodes. They proposed cross-linking modification of PEDOT:F by introducing polyethylene glycol diglycidyl ether (PEGDE) (Figure 3). The cross-linked c-PEDOT:F film forms an ethanol-resistant network structure through chemical bonding, significantly enhancing its resistance to solvent penetration while maintaining a high work function (~ 5.5 eV) and suitable conductivity. A flexible organic solar cell (OSCs) based on this cross-linked layer was developed [12]. Achieved a small-area efficiency of 14.86% (0.041 cm^2), which is 1.15% higher than that of uncrosslinked devices. The further prepared flexible module with an area of 21.18 cm^2 achieved an efficiency of 12.38%, demonstrating the effectiveness of this strategy in large-size devices. This study provides a new approach to addressing the compatibility issues of functional layers in solution-processed flexible OSCs [13].

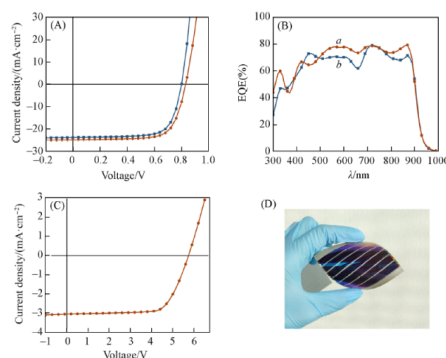


Figure 3: The synergistic effect of PEGDE additives on the performance optimization of organic solar cells and the development of flexible components. (A) J-V characteristics; (B) EQE spectra of small-area top-illuminated OSCs with (a) and Without (b) 0.05% PEGDE; (C) J-V characteristics; and (D) a picture of the fabricated 21.18 cm^2 flexible organic solar module [13]

Flexible and transparent photovoltaic materials face three core challenges in application and promotion: stability, large-scale production and environmental friendliness. In terms of stability, the perovskite light-absorbing layer is prone to crystal boundary defects due to bending, and flexible electrodes [14]. The fatigue resistance of materials like ITO is insufficient, and their sensitivity to water and oxygen leads to a decline in long-term reliability. Large-scale production is hindered by the need for uniform film control, the immaturity of flexible packaging technology, and the high cost of high-performance conductive films. Environmental friendliness is constrained by the lead toxicity in perovskite materials, the dependence on rare metals (like ITO), and the difficulty in recycling multi-layer structures. Balancing efficiency improvements with ecological sustainability is essential.

4. Conclusion

This paper highlights the pivotal role of nanomaterials in advancing next-generation photovoltaic (PV) technologies, focusing on key applications and challenges. Despite remarkable efficiency gains in emerging PV systems like perovskite, quantum dot, and organic solar cells, commercialization remains hindered by stability issues, scalability limitations, and environmental toxicity. Three primary innovation pathways are explored: metamaterials / metasurfaces, which leverage engineered nanostructures to enhance light manipulation and device miniaturization; single-atomic-layer materials, offering atomically thin structures with high surface activity for catalysis and interface engineering; and flexible/transparent PVs, combining lightweight, bendable designs with semi-transparent electrodes for multifunctional applications.

Critical challenges across these domains include ensuring long-term stability under operational conditions, achieving cost-effective mass production, and transitioning toward eco-friendly materials. For metamaterials, structural degradation and high manufacturing costs pose barriers; single-atomic-layer materials struggle with mechanical sensitivity and synthesis scalability; while flexible/transparent PVs face issues like fatigue-induced defects, lead toxicity, and complex recycling.

Future research must prioritize stability-efficiency synergy, sustainable synthesis methods, and cross-disciplinary innovations to balance performance, cost, and environmental impact. This evolution is crucial for realizing affordable, durable, and green PV technologies aligned with global decarbonization goals.

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