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*Original Research Article*

# Nanomaterial-Enabled Strategies for High-Performance and Stable Perovskite Solar Cells

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## ABSTRACT

Perovskite solar cells have attracted significant attention in recent years due to their rapidly rising power conversion efficiencies and low-cost fabrication potential, and the incorporation of nanomaterials provides new pathways to further improve their performance and stability. In this work, the structure of the perovskite solar cell is first introduced, accompanied by the function of the buffer layer, the perovskite photosensitive layer, and the electrode. The advantages and drawbacks are analyzed by employing diverse nanomaterials in the three critical regions of perovskite solar cells. The enhanced performance is discussed in terms of the buffer layer, the perovskite photosensitive layer, and each component with the incorporation of nanomaterials, and the underlying mechanisms are examined to reveal how nanomaterials improve photoelectric conversion performance. In perovskite solar cells, nanomaterials play a critical role by passivating defects, suppressing electron–hole recombination, accelerating charge separation, and enhancing carrier transport, thereby improving device efficiency and stability. This study provides insights into the rational design of nanomaterial-based strategies to further advance the development of high-performance and stable perovskite solar cells.

## KEYWORDS

*Nanomaterial, Perovskite solar cell, Electron transfer efficiency, Photoelectric conversion, Surface passivation.*

## INTRODUCTION

The growing threat of global climate change has led international organizations to increase policy support for energy transition and carbon reduction. The 2022 United Nations Climate Change Conference (COP27) emphasized the need for a balanced global strategy, including both a just transition and effective climate adaptation. Concurrently, policies such as the EU

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Green Deal and the U.S. Inflation Reduction Act (IRA) have provided unprecedented financial and regulatory support for renewable energy technologies. The development of clean energy and the improvement of energy efficiency have become central pillars of global energy policy.

Solar energy has become a pivotal driver of the global energy transition owing to its abundant availability and environmental advantages. In particular, photovoltaic (PV) technologies have seen rapid advancements in recent years. Perovskite solar cells (PSCs), characterized by high efficiency, low production cost, and compatibility with solution processing, have quickly risen to prominence as a next-generation PV technology [1]. Although PSCs initially exhibited power conversion efficiencies (PCEs) of only 3 % – 5 %, continuous development over the past decade has pushed PCEs beyond 23 %. However, the commercialization of PSCs is limited by the poor device stability, extensive interfacial defects, and severe charge recombination. In addition, the cell materials are prone to degradation under prolonged exposure to sunlight and humid conditions, along with the potential environmental risks. Innovative technological solutions are urgently needed to enhance the performance of PSCs [2].

Generally, the PSCs consist of a perovskite photoactive layer, two buffer layers, and electrodes. The construction of PSCs is shown in **Figure 1**. The buffer layer is usually composed of an electron transport layer (ETL) dominated by n-type semiconductors and a hole transport layer (HTL) dominated by p-type semiconductors. ETL and HTL are distributed on both sides of the perovskite in the PSC. Functional nanomaterials integrated into the various layers of PSCs play a pivotal role in boosting light absorption, optimizing charge extraction, and mitigating defect-induced recombination, which directly translates into higher efficiency and improved device stability. For example, plasmonic metal nanoparticles (NPs) can enhance light absorption and hot electron generation in semiconductors [3]. Carbon-based nanomaterials modulate the electrical properties of the device, contributing to improved device longevity and degradation resistance due to their chemical stability and compatibility with perovskite layers [4]. Metal–organic framework (MOF) materials can optimize energy level alignment, fill interfacial defects, and reduce recombination processes through interfacial engineering [5]. Additionally, emerging nanomaterials such as two-dimensional materials and quantum dots exhibit significant potential for controllable integration into PSC architectures, offering valuable opportunities for further research.

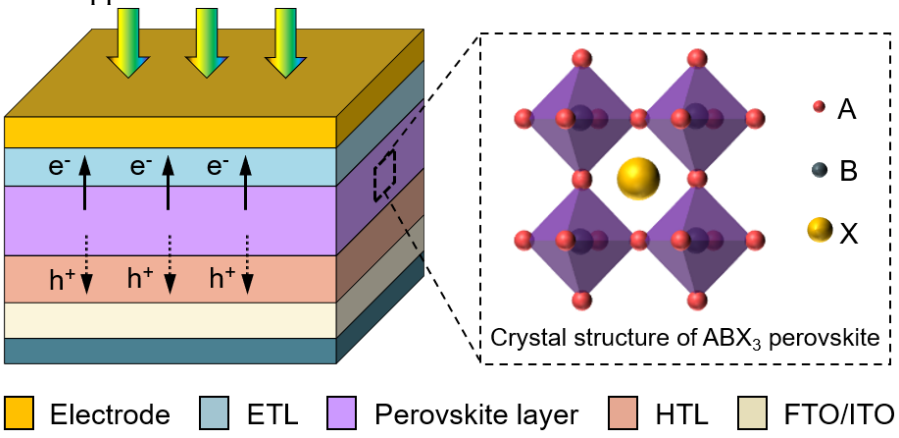


Figure 1. Construction of a perovskite solar cell

However, a clear knowledge gap remains despite substantial progress and several existing review articles. Some reviews primarily provide broad discussions on PSC development trends and general technical challenges, but lack in-depth mechanistic analysis of how specific nanomaterials function within each device layer or influence operational physics [3,6]. Other reviews focus on only one or two classes of nanomaterials, such as plasmonic nanoparticles, carbon nanostructures, or MOF materials, without offering a comprehensive comparison across material categories or explaining their synergistic roles throughout the ETL, perovskite, HTL,

and electrode interfaces [7,8]. Critically, no existing work systematically correlates nanomaterial properties with device-level performance enhancement in a layer-by-layer framework, nor do they unify synthesis strategies, interfacial mechanisms, and stability considerations into an integrated perspective.

To address this gap, this review provides a systematic and comparative analysis of nanomaterials used across all functional layers of PSCs. It summarizes the mechanisms by which different nanomaterials improve charge transport, defect passivation, optical management, and structural stability. Furthermore, it highlights their relevance to flexible PSC architectures and long-term operational durability. The review concludes by identifying unresolved challenges and outlining future research opportunities, offering both theoretical guidance and practical insights for the rational design and integration of nanomaterials in next-generation perovskite solar cells. In this study, a systematic literature search was conducted using Web of Science over the period 2013-2025. The search employed combinations of the keywords "nanomaterials", "perovskite solar cells", and related terms. In total, 103 publications were retained for detailed analysis after screening titles, abstracts, and full texts according to their relevance to the research topic.

## THE STRENGTHENING MECHANISM OF NANOMATERIALS

The symbol efficiency (the highest efficiency in that year) breakthrough of PSCs is shown in Figure 2. Since the first application of perovskite materials in solar cells, the photoelectric conversion efficiency has increased from 4 % [9] to 25.7 % [10]. Nanomaterials play important roles in the improvement of photothermal efficiency.

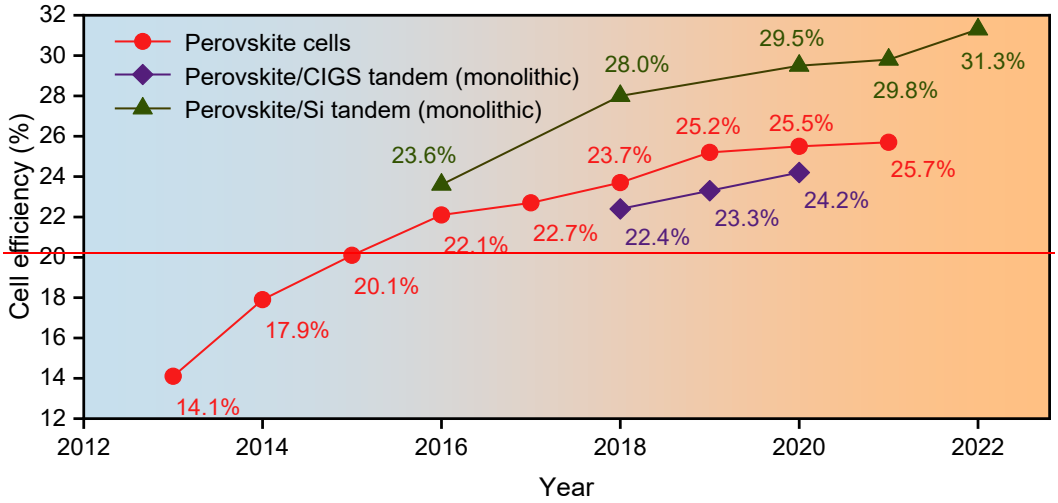


Figure 2. Best research-cell efficiencies of perovskite solar cells (from US-NREL [11])

### Defect Passivation

Perovskite layers and charge-transport layers inherently contain trap states that induce non-radiative recombination. Nanomaterials act as efficient passivators by chemically coordinating under-coordinated ions, compensating halide vacancies, or forming ultrathin interlayers that screen interfacial defects. For instance, MXene-modified ETLs, carbon-nanodot-based interlayers, and $CuInSe_2$ quantum-dot additives have all been reported to lower trap densities at ETL/perovskite interfaces or within perovskite films, thereby improving crystal quality, extending carrier lifetimes, and suppressing non-radiative recombination [12,13].

### Charge Transport Enhancement

Slow charge transport and interfacial energy-level mismatch limit charge extraction efficiency in PSCs. Nanomaterials can be engineered into ETLs, HTLs, or perovskite absorbers to increase carrier mobility, optimize band alignment, and introduce beneficial interfacial dipoles, thereby accelerating charge extraction and suppressing interfacial recombination.

Representative strategies include high-mobility oxide nanowires as ETLs, core-shell nanorod arrays as HTLs, and doped NiO nanoparticles that form interfacial dipoles with transparent electrodes, all of which have been shown to enhance charge-collection efficiency and open-circuit voltage [14,15].

### Light Absorption Optimization

Nanomaterials can extend and intensify light harvesting in PSCs through plasmonic enhancement and light-trapping architectures. Plasmonic metal nanoparticles embedded in transport layers or perovskite films generate localized surface plasmon resonance (LSPR) that strengthens the local electromagnetic field and increases absorption within the perovskite layer [16], In parallel, nano-textured interfaces such as prisms, core-shell nanorod arrays, and hexagon-like patterns on transparent electrodes increase the optical path length via multi-directional scattering and reflection, thereby improving photocurrent and power conversion efficiency compared with planar counterparts.

### Stability Improvement

Environmental stressors such as moisture and prolonged illumination accelerate perovskite degradation. Nanomaterials can improve device stability by providing physical encapsulation and chemical stabilization. Copper-based inorganic nanocrystals used as HTLs offer higher moisture resistance than conventional organic counterparts, thereby slowing performance decay. Carbon nanomaterials introduce hydrophobic, conductive barriers at the perovskite/HTL interface, effectively blocking moisture ingress while maintaining charge transport.

It should be noted that the four roles discussed above, defect passivation, charge-transport enhancement, light-absorption optimization, and stability improvement, are often strongly coupled rather than strictly independent. In many cases, a single nanomaterial simultaneously passivates interfacial traps, tunes energy-level alignment, modifies the local optical field, and alters the device resistance to moisture or ion migration. Conversely, strategies that focus on one aspect (e.g., introducing plasmonic nanoparticles for stronger light harvesting) may inadvertently affect others, such as interfacial recombination or long-term stability.

## THE APPLICATION OF NANOMATERIALS IN THE PEROVSKITE SOLAR CELL

In this section, the use of nanomaterials in different functional regions is comprehensively reviewed, with a comparative evaluation of their effects. A systematic discussion of the mechanisms underlying the enhancement of photoelectric conversion efficiency is conducted, focusing on the buffer layer, the perovskite photosensitive layer, and the electrode.

### Buffer layer with nanomaterials

*Electron transport layer* Widely used $TiO_2$ [17], ZnO [18], and $SnO_2$ [19], the electron transporting layer has essential functions of improving the extraction efficiency of photoelectrons and blocking the migration of holes toward the cathode. Energy level, aperture size, and electron mobility are mostly controlled based on various preparations [20], morphology [21], and doping methods [22,23], and the cell performance caused by the factors is shown in Figure 3. The electron transfer efficiency is improved by doping nanomaterials, such as Zr-doped $TiO_2$, Mg-doped $TiO_2$, $Li^+$-doped $BaTiO_3$, Al-doped ZnO, Cd-doped ZnO, boron-doped ZnO, Cu-doped $SnO_2$, $Na^+$-doped $SnO_2$, $TaC_{15}$-doped $SnO_2$, Sb-doped $BaSnO_3$, etc. For the passivation of surface defects, nanoflakes $Ti_3C_2T_x$ MXene reduce the defect density from $5.65 \times 10^{15}$ to $2.25 \times 10^{15}$ $cm^{-3}$ for the $SnO_2$ electron transport layer [12]. It is proven that the improvement in conversion efficiency is mainly due to the passivation of electronic defects instead of the modification in charge transfer at the interface [23].

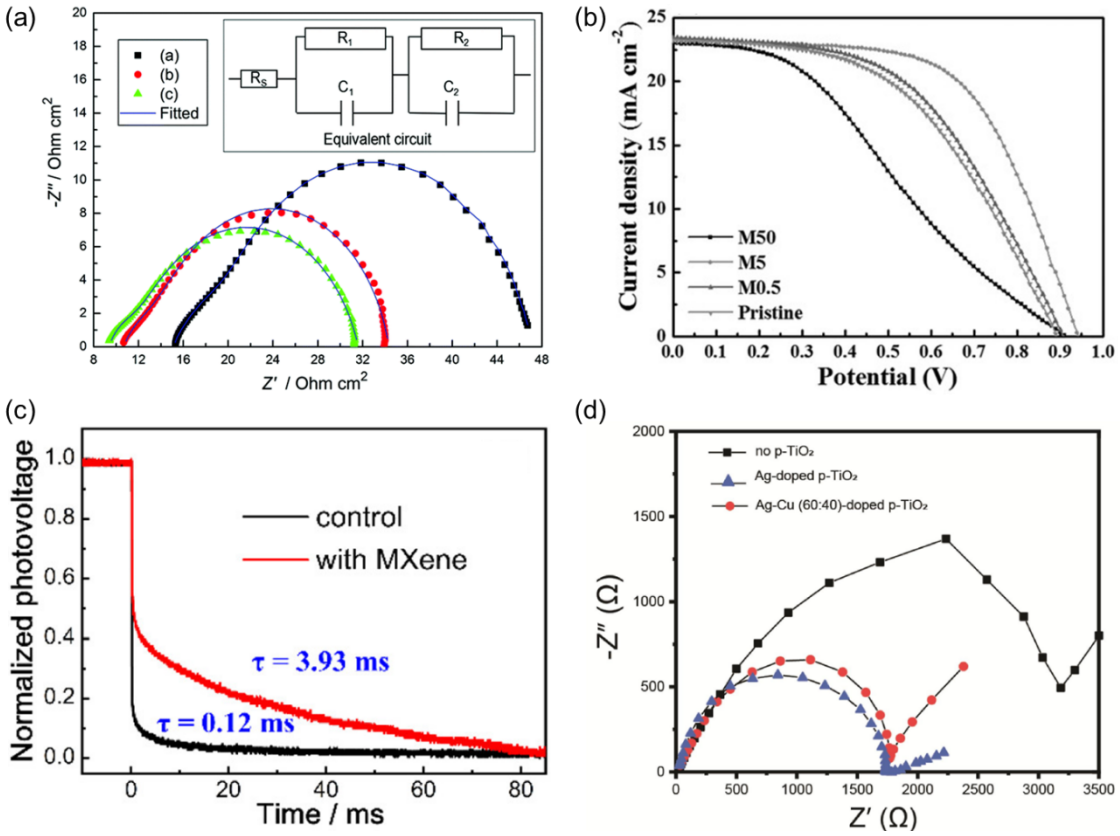


Figure 3. Influence of preparation methods and nanoparticle attachment on the performance of perovskite solar cells: (a) Electrochemical impedance spectra (EIS) fitted with equivalent circuit models for devices prepared by different methods [20]; (b) J–V characteristics of perovskite solar cells prepared under different processing conditions [21]; (c) Transient photovoltage decay showing charge carrier lifetime with and without MXene nanoparticles [22]; (d) Electrochemical impedance spectra of devices with pristine, Ag-doped, and Ag–Cu co-doped $TiO_2$ layer [23]

Insulating oxides, such as $Al_2O_3$, $ZrO_2$, and $SiO_2$, are usually used for electron transporting to replace the mesoporous titanium dioxide in perovskite solar cells. Semiconductor oxides, such as $SrTiO_3$, $WO_3$, and $SnO_2$, are also used as substitutes for compact $TiO_2$. The electron mobility of $SrTiO_3$ is higher than that of $TiO_2$ at room temperature. The ferroelectric effect of $SrTiO_3$ effectively weakens the electron recombination at the interface for a high open-circuit voltage [14]. $WO_3$ with a narrow band gap, high carrier mobility, and nanostructure fabrication results in an excellent photoelectric conversion efficiency [24]. Employing a bilayer structure in the electron transport layer enables the integration of complementary advantages from distinct materials, thereby overcoming the weaknesses associated with single-component systems. The electron-transporting layer with a bilayer structure shows excellent carrier transmission characteristics, indicating a significant energy level difference between the perovskite layer. Usually, nanoparticle-based mesoporous and blocking layers achieve highly efficient charge collection [25].

Several criteria are considered to determine whether a material is suitable for an electron transport layer, such as energy level matching, electron injection, and electronic transmission. Pores or holes are formed due to the rigid structure when the metal oxide is used as an electron-transporting layer. Nanomaterials can be in close contact with perovskite crystals to reduce leakage. The selection of materials for electron transport increases by doping nanoparticles and nanostructure design. The effects and mechanisms of nanomaterials in the electronic transport layer are summarized in Table 1.

Table 1. Nanomaterials in the electron transport layer (ETL)

| Nanomaterial | Mechanism | Effect Size | Processability | Cost | Reference |
|---|---|---|---|---|---|
| ZnO (doped with Al, Cd, B) | Boost electron extraction, tune band alignment | Leakage current reduced; charge separation efficiency | Low-temperature processable; easy to synthesize as thin films | Low | [18] |
| $SnO_2$ (doped with Cu, $Na^+$, $TaCl_5$) | Enhance electron transport speed, suppress charge recombination | $Na^+$ doping reduces trap states; carrier mobility higher than $TiO_2$ | Aqueous sol-gel process; no high-temperature annealing required | Low | [19] |
| $TiO_2$ (doped with Zr, Mg, $Li^+$, Ag-Cu) | Optimize energy levels, block hole migration, passivate surface defects | Ag-Cu co-doping reduces interfacial resistance; electron transfer efficiency enhanced | Mature solution-processable; compatible with existing fabrication lines | Low | [23] |
| $Ti_3C_2Tx$ MXene Nanoflakes | Passivate defects, reduce charge trapping | Defect density reduced from $5.65\times10^{15}$ to $2.25\times10^{15}$ $cm^{-3}$; carrier lifetime extended to 3.93 ms | Complex exfoliation process; requires precise control of layer thickness | Medium | [12] |
| $SrTiO_3$ | Ferroelectric effect suppresses interfacial recombination; replace $TiO_2$ | Room-temperature electron mobility higher than $TiO_2$; open-circuit voltage increased | Difficult nanostructuring; high-temperature sintering required | Medium | [14] |
| $WO_3$ | Narrow bandgap enhances light response; high carrier mobility | Photoelectric conversion efficiency significantly improved | Facile nanostructure fabrication via template methods | Medium | [24] |

Hole transport layer. Hybrid perovskite materials transport electrons and holes. Without a hole transport layer, perovskite solar cells have achieved high photoelectric conversion efficiency [26]. This design completes the simplification of manufacturing and the reduction in costs. However, the hole transporting layer prevents the quenching effect caused by the direct contact between the perovskite layer and the electrode completely. This quenching effect is challenging to overcome for PSCs without an HTL. The hole transport layer is used to ensure the stability of perovskite materials in moisture [27].

Inorganic [28] and organic materials [29] are used in the hole transport layer. Organic Spiro-OMeTAD is extensively used as an organic hole transporting material in perovskite solar cells. Due to the difficulty of the Spiro-OMeTAD purification, the triphenylamine polymer with lithium electrolyte salt (Li-TFSI) is used as the hole-transport material in perovskite solar cells. Perovskite materials are easily destroyed due to the moisture absorption of the Li-TFSI. This problem is effectively alleviated by the functionalized Spiro-OMeTAD solid hole

conductor, and photoelectric conversion efficiency of 24.82 % is obtained using the fluorinated isomeric analogs of the stable Spiro-OMeTAD [30], as shown in Figure 4.

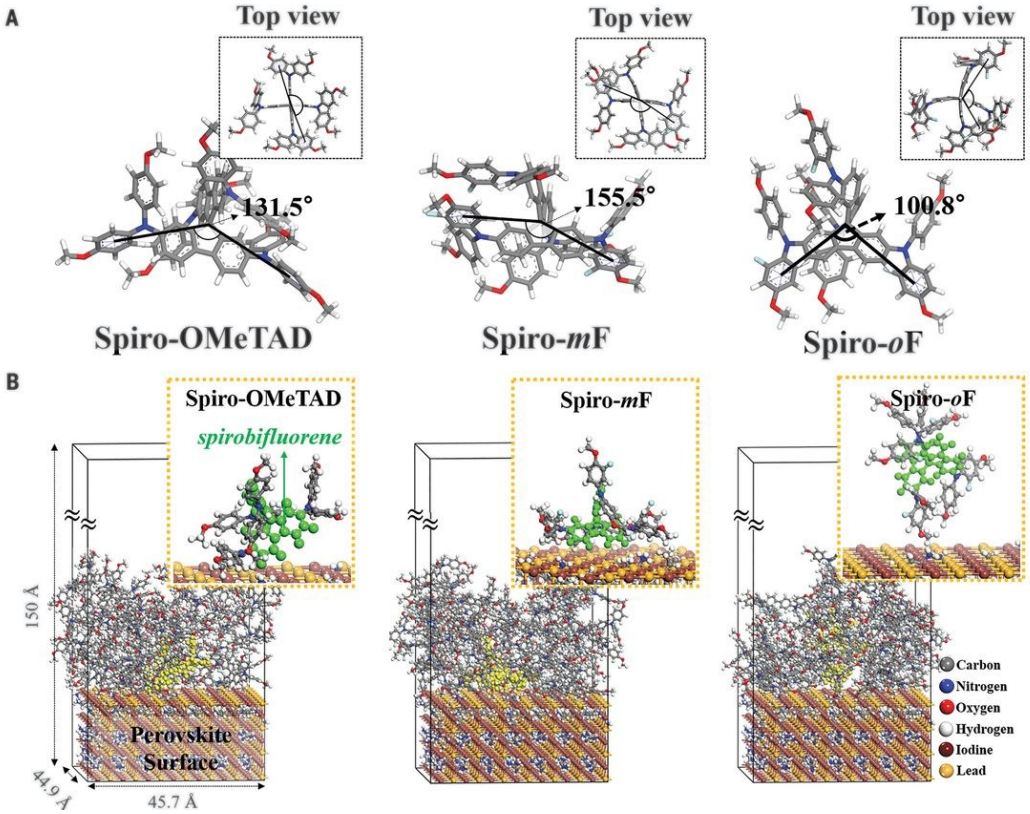


Figure 4. Molecular simulations: (A) Optimized molecular structure of Spiro-OMeTAD, Spiro-mF, and Spiro-oF; (B) Adsorption structures of Spiro-OMeTAD, Spiro-mF, and Spiro-oF on the surface of perovskite [30]

Compared with traditional organic-hole transport materials, inorganic materials have better chemical stability, higher hole mobility, and lower synthetic costs. Nickel oxide (NiO) possesses a hole mobility of 47.05 $cm^2 \cdot V^{-1} \cdot s^{-1}$, which nicely matches the energy level of perovskite materials by autoregulation. The morphology control of nickel oxide fabricates the light trapping scheme quickly. The NiO@GeSe core-shell nano-rod (NR) array causes a reduction of carrier recombination within the perovskite solar cells [15]. $NiO_x$ fibers address the poor interface quality in PSCs [31]. $NiO_x$ nanoparticles are modified with poly(vinyl alcohol) to improve the contact between $NiO_x$ and perovskite [32]. Doping nanomaterials offsets some degradation in performance due to the $NiO_x$ pretreatment. Electrical conductivity is enhanced by doping Zn [33] or CNT [34], and surface roughness decreases by doping Ce. An interfacial dipole is found between the ITO electrode and the Al-doped $NiO_x$ nanoparticles (NPs) layer, which improves the hole extraction efficiency at the ITO/$MAPbI_3$ (MA = methylamine) interface [35].

Inorganic copper-based semiconductors such as CuSCN have good hydrophobicity, high transparency, and outstanding optoelectronic properties as hole transport layers [36]. The polar solvents in the preparation process are liable to the degradation of the perovskite materials with time. In order to solve this problem, reductive graphene oxide is prepared as intermediates or bilayers to avoid direct contact between the perovskite layer and polar solvents. The electrical conductivity of copper-based materials is improved by reduced graphene oxide (RGO) [37]. In addition, copper-based nanocrystals have been confirmed to be more stable in moisture than the organic materials Spiro-OMeTAD and NiO [38]. Alloyed quantum dots $(Cu_2SnS_3)_x(ZnS)_{1-x}$ as a hole transporting layer achieves suitable energy level alignment between perovskite layers [39]. The effects and mechanisms of nanomaterials in the hole transport layer are summarized in Table 2.

Table 2. Nanomaterials in the hole transport layer (HTL)

| Nanomaterial | Mechanism | Effect Size | Processability | Cost | Reference |
|---|---|---|---|---|---|
| Fluorinated Spiro-OMeTAD Derivatives (Spiro-mF, Spiro-oF) | Suppress moisture absorption; optimize perovskite surface adsorption | PCE up to 24.82 %; voltage loss reduced by 0.3 V | Complex purification process; solid-state processing required | High | [30] |
| NiO (doped with Zn, CNT, Ce; NiO@GeSe core-shell NRs) | Enhance hole mobility; reduce surface roughness; suppress recombination | Hole mobility = 47.05 $cm^2V^{-1}s^{-1}$; Ce doping lowers surface roughness | Low-temperature sol-gel process; PVA modification improves film uniformity | Low | [15,33] |
| Cu-based Semiconductors (CuSCN, $CuInS_2$, RGO-modified CuO) | Hydrophobic protection; improve conductivity; block moisture | More stable in humidity than Spiro-OMeTAD; RGO doping boosts conductivity | CuSCN solution-processable; RGO composite requires dispersion control | Low | [37,38] |
| Alloyed Quantum Dots $(Cu_2SnS_3)_x(ZnS)_{1-x}$ | Tune energy level alignment; passivate interfacial defects | Perovskite-HTL band matching optimized; recombination reduced | Hot-injection synthesis; easy to tune composition | Medium | [39] |

**Perovskite photosensitive layer with nanomaterials**

Perovskite materials in optoelectronic devices absorb incident light, generate and transport electrons and holes. In order to achieve the effective absorption of the incident light, the power conversion efficiency is increased by improving the energy band structure of the solar cells [40]. The migration and recombination of electrons and holes are affected by properties of perovskite materials, such as exciton binding energy, carrier mobility, density, and distribution of trap states. The stability of perovskite material is also a crucial factor in the overall performance of PSCs. Nanomaterials in PSCs achieve high absorption of incident light by adjusting the band gap, constructing a light-trapping configuration, and exciting the surface plasma effect. The presence of nanoparticles is conducive to forming the perfect lattice structure of perovskite material for improvements in carrier transport and stability performance.

The localized surface plasmon resonance of nanoparticles has enhanced induced light absorption and carrier separation. Plasmonic enhancements in PSCs are closely related to the morphology, size, composition, and structure of meta-nanoparticles [41]. Different distribution, additive quantity, and embedding depth of Ag nanoparticles result in absorption differences in various spectrums [16,42,43], as shown in Figure 5. Composite nanorods Au/Ag@CuSCN are developed to absorb solar radiation at a wavelength of 500 - 800 nm [44]. Plasmonic wavelengths cover the visible light region by adjusting the sizes and shapes of plasmonic nanoparticles and shell thicknesses [45]. Hexagon-like nanostructures located on the backside of conductive glass (indium tin oxide-ITO) enhance the scattering and gathering of light in the ultraviolet-visible (UV-Vis) spectrum [46]. The light response of plasmonic Au nanorods (NRs) is improved in the NIR region [47], but Zheng et al. [48] declared that the enhancement

of light absorption is negligible due to the localized surface plasmon resonance (LSPR) and light scattering of Au nanoparticles. Although low-cost Cu nanoparticles also conduct the localized surface plasmon resonance, these Cu nanoparticles are rarely used in PSCs due to their accessible oxidation property [49].

After being struck by the light-trapping configuration, the optical path in solar cells increases the incident light due to absorption, reflection, and refraction. The nano-textured structure achieves over 30.48 % enhancement in power conversion efficiency compared to the planar structure in PSCs [50]. The conventional light-trapping nano-prisms [51] and nano-pyramids [52] have been applied in the perovskite photosensitive layer. The appropriate preparation of nanomaterials improves the optical absorption property. For example, the plasmonic core/shell nanorod (PLCS-NR) array combined light-trapping structure and surface plasma resonance for excellent light absorption [44]. Besides achieving efficient light capture, a light-trapping-configuration hole/electron transport layer is beneficial to the separation of electrons and holes, the simplification of the preparation process, and the reduction of cell thickness [15,53,54]. The textured substrate for ultra-thin perovskite solar cells significantly enhances the light-trapping, separation, and collection of photo-generated charges [54]. Due to the complex technological process of nanomaterial synthesis and the high-cost machining of nanostructures, the published studies show the improvement of photoelectric conversion performance mostly using conventional nanoscale light-trapping structures numerically.

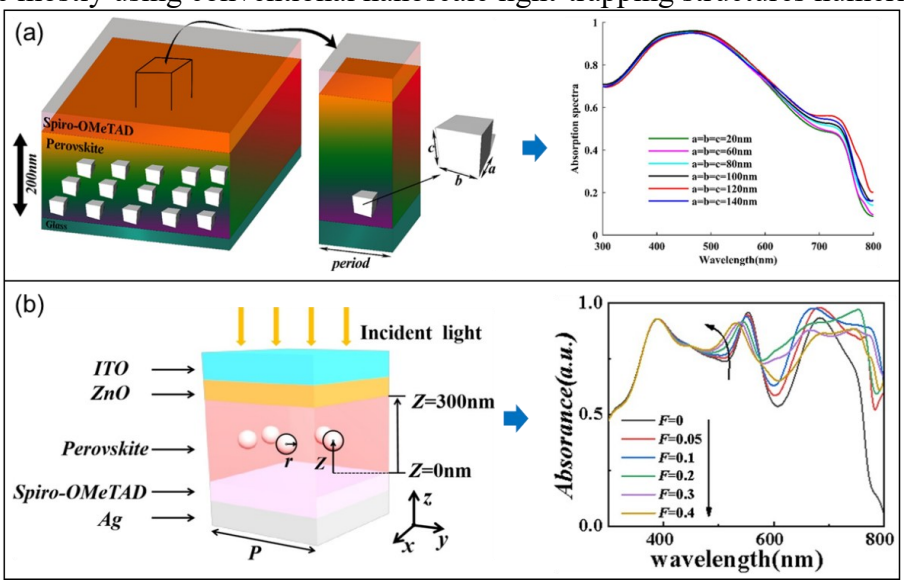


Figure 5. Absorption spectra of the perovskite solar cell with Ag nanoparticles: (a) Particle size [16]; (b) Particle concentration [42]

Perovskite crystallinity and morphology are central to ensuring the high photovoltaic performance of devices. For the conventional perovskite film crystallization with additives in the synthesis process [55,56], the morphological characteristics of additives are beneficial in providing more chemical anchor sites [57]. Additives are often introduced into perovskite precursors as a solution to control nucleation [58], to slow down the crystallization rate [59,60], and to intensify the preferred orientation of crystals. Usually, organic compounds are used as additives. The function of nanomaterials on crystallization control is achieved based on interface engineering. As a scaffold layer between the compact $TiO_2$ layer and the perovskite layer, the lead-containing metal-organic framework (Pb-MOF) provides nucleation points to promote perovskite crystallization [61]. The perovskite morphology is improved using the $TiO_2$ network as the electron transporting layer (ETL) [62,63], which contributes to favorable junctions between the perovskite photosensitive layer and electron transport layer. Natriumion-functionalized carbon nanodots (CNDs@Na) interlayer improves perovskite ordering, crystal size, and interfacial contact [13]. With a hot injection method, the nanodots are also introduced into the perovskite to passivate trap states [64]. The growth of crystalline perovskite films is

controlled by the seed-mediated techniques with nanoparticles. $SiO_2$-coated Au/Ag-alloyed nanoprisms [65], $GeO_2$ nanoparticles [66], ZnO nanoparticles [67] have been used as inducers for fast nucleation in the seed-mediated techniques. The mechanisms of nanomaterials in the perovskite photosensitive layer are summarized in Table 3.

Table 3. Nanomaterials for the perovskite photosensitive layer

| Nanomaterial | Mechanism | Effect Size | Processability | Cost | Reference |
|---|---|---|---|---|---|
| Plasmonic NPs (Au, Ag, Au/Ag@CuSCN) | Localized surface plasmon resonance (LSPR); enhance light absorption/charge separation | Absorbs 500–800 nm solar radiation; Au nanorods improve NIR response | Core-shell NPs require multi-step synthesis; Ag NPs easy to disperse in precursors | High | [44,47] |
| Nano-textured Structures (nanoprisms, nanopyramids, PLCS-NR arrays) | Construct light-trapping configurations; extend optical path | PCE enhanced by >30% vs. planar structures | Complex machining (e.g., nano-imprinting); high precision required | Medium | [50] |
| Pb-MOF, CNDs@Na | Induce perovskite nucleation; passivate trap states; improve crystallinity | Perovskite crystal size increased; defect density reduced | Pb-MOF requires ligand coordination; CNDs@Na easy to disperse in precursors | Medium | [13,61] |
| $GeO_2$, ZnO NPs | Seed-mediated fast nucleation; suppress pinhole formation | Pinhole-free perovskite films; crystallization rate accelerated | Easy to integrate into precursor solutions; low-temperature compatible | Low | [66,67] |

**Electrode with nanomaterials**

Although the indium tin oxide (ITO) electrode in the scalable PSCs is an excellent conductive material for the stable performance of devices [68], the brittleness of the ITO electrode has limited the progress of PSC commercialization. Recently, flexible PSCs have attracted well-deserved attention, and they are a large-area production using roll-to-roll manufacturing [69]. Flexible perovskite solar cells (F-PSCs) suffer from low power conversion efficiency (PCE) compared to rigid PSCs [70,71]. PSCs have certified PCEs of 25.6 % and 24.4 % on rigid conductive substrates [10] and flexible substrates [72]. To fabricate high-efficiency flexible perovskite solar modules (PSMs), it is essential to develop a robust and reliable flexible electrode [73]. Flexible substrates are made of polyester plastic, conductive cloth [74], metallic titanium [75], and cellophane paper [76]. The flexible polyester plastic substrate with high light transmittance offers a possibility for manufacturing flexible transparent electrodes. A thin layer of metal nanoparticles, metal nanowires, and carbon nanomaterials is mostly used to synthesize flexible substrates as flexible electrodes.

Prepared with carbon materials, flexible electrodes demonstrate superior robustness against mechanical deformation. With the advantage of structure, carbon nanotubes and graphene nanosheets show excellent performance in electrical conduction. At room temperature, electron mobility achieves $2\times10^5$ $cm^2 \cdot V^{-1} \cdot s^{-1}$ and $1\times10^5$ $cm^2 \cdot V^{-1} \cdot s^{-1}$ for carbon nanotubes and graphene nanosheets. These properties contribute to machining ultrathin, lightweight, and flexible

perovskite solar cells with graphene transparent electrodes [77]. A manufacturing method has been reported for the monolayer graphene-based large-scale flexible electrode [78]. The number of graphene layers is determined based on a balance correlation among structural, optical, and electrical properties of the solar cells [79]. Although carbon nanotubes have lower transmittance than graphene nanosheets, films of a carbon nanotube network meet the requirement of semi-transparent perovskite solar cells [80]. Compared with graphene nanosheets, CNTs in the electrodes as additives improve charge extraction more efficiently due to the morphological feature of overlength fibers [81].

Metal films with a thickness above 15 nm show high uniformity and conductivity, but the metal films above 15 nm cannot meet the requirements of transparent electrodes. The transmissivity and square resistance of metal films are constrained by each other. The metal films between dielectric materials with a high refractive index are introduced to fabricate the flexible transparent electrodes. As flexible transparent electrodes, each layer of oxide/metal/oxide (OMO) film has a specific thickness requirement for high transmission coefficients, high electrical conductivity, low roughness, long-term stability, and outstanding bending-proof performance [82,83]. The flexible electrodes are fabricated with various OMO structures, such as ITO/Ag/ITO [84], ZnO/Au or Ag/ZnO [85], NiO/Ag/NiO [86], $TiO_2$/Ag/$TiO_2$ [76], and $SnO_2$/Ag/$SnO_2$ [87]. Metal materials Ag and Au are mainly used as intermetallic layers of OMO films. The high malleability of material Ag is liable to improve transparency. Traditional metallic films are replaced with metallic grid patterns [88].

With excellent electrical and optical properties, silver nanowires (NWs) provide localized channels for charge carrier transport in the Ag-NWs flexible electrodes [89]. Applications of Ag NWs in high-performance PSCs are limited by large surface roughness, migration of Ag, and chemical reaction between Ag and perovskite precursors. Some measures are recommended to overcome these limitations, including the introduction of anti-corrosion additives into electron transport layers [90], in combination with the low-temperature sol-gel oxide [91], employing solution-deposition of conductive nanoparticles [92], and synthesis of a physical separation shell for Ag NWs [93]. Solution-processed nanofiller generates a high contact area and favorable energy level alignment at the interface between the electron transporting layer and the nanowire-based flexible electrode [94]. By one-step doctor-blade-coating processing, the transparent electrode of Ag-NWs-ZnO-polyethylenimine ethoxylated composite films also serves the function of electronic transportation [95]. The PSCs with flexible nanowire electrodes show a similar power conversion efficiency to the commercial flexible solar cells with ITO electrodes, but the nanowire-based substrate shows more excellent flexibility and stability than the ITO-based PSCs [88]. Besides silver nanowires, copper nanowires are used as additives for flexible electrodes [96-98]. However, the thermal stability and oxidation resistance of Cu nanowires are significantly lower than those of Ag nanowires. The current density of the perovskite solar cells with different flexible electrodes is compared in Figure 6. It is recommended to use Ag nanowires as electrode materials for flexible perovskite solar cells. The roles of nanomaterials in the perovskite photosensitive layer are summarized in Table 4.

## CONCLUSIONS

Nanomaterial-based strategies offer critical technical support for the iterative optimization of perovskite solar cells (PSCs) and address the core contradiction among performance, stability, and processability. In terms of structural optimization, they enable precise regulation of interface contact, defect density, and charge transport paths in PSCs, providing engineering-oriented solutions. For performance breakthroughs, leveraging technologies such as plasmonic enhancement, they overcome the performance bottleneck of traditional PSC structures, with the power conversion efficiency (PCE) of relevant PSCs improving by over 30 % compared to planar structures.

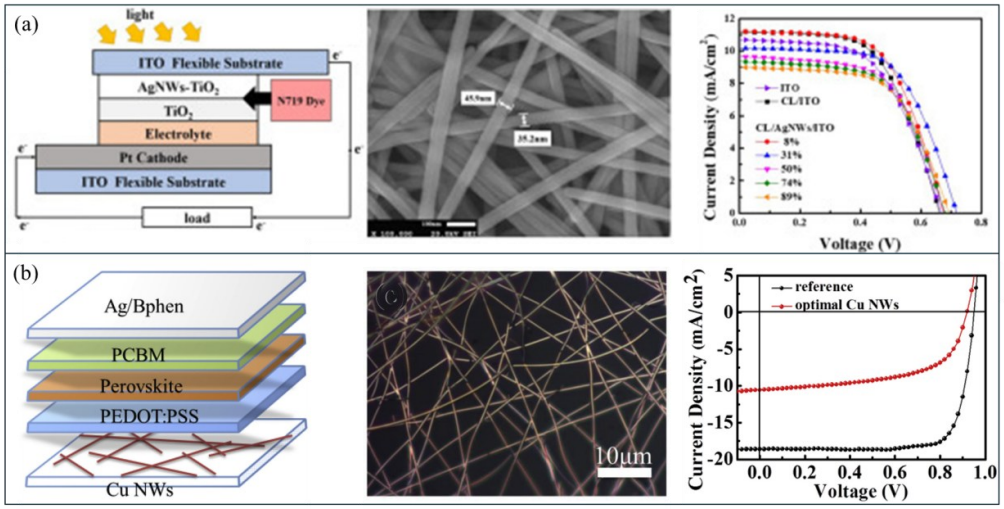


Figure 6. The photoelectric conversion performance of flexible perovskite solar cell with different electrode materials: (a) Ag nanowire [90]; (b) Cu nanowire [91]

Regarding process simplification, they promote the development of simplified architectures, including hole transport layer-free (HTL-free) PSCs and Ag-NWs-ZnO composite electrodes fabricated via one-step doctor-blade coating, which simplifies the fabrication process while maintaining high efficiency, laying a solid foundation for the low-cost manufacturing of PSCs. The integration of nanomaterials bridges the gap between laboratory-scale PSC research and industrialization, with broad application prospects in multiple scenarios. Some main conclusions are summarized as follows:

1) For harsh environmental scenarios featuring high humidity and prolonged illumination, materials including $Ti_3C_2T_x$ MXene nanosheets, reduced graphene oxide (RGO), lead-based metal-organic frameworks (Pb-MOFs), and oxide/metal/oxide (OMO) structured materials are required to achieve moisture barrier capability, defect passivation, and crystal structural stability.
2) For flexible application scenarios demanding bendability and large-area roll-to-roll fabrication, nanomaterials such as carbon nanotubes (CNTs), graphene nanosheets, and silver nanowires (Ag NWs) integrate high electrical conductivity, mechanical toughness, and compatibility with large-scale manufacturing processes, exhibiting power conversion efficiency comparable to that of traditional indium tin oxide (ITO) electrodes.
3) In high-efficiency light absorption scenarios targeting broad spectral response and elevated light utilization efficiency, silver nanoparticles (Ag NPs), Au/Ag@CuSCN composite nanorods, and nanoprisms enhance the absorption of visible and near-infrared (NIR) light through the localized surface plasmon resonance (LSPR) effect and optical path extension design.
4) For low-defect and high-carrier transport scenarios aimed at mitigating carrier recombination and improving device efficiency, Zr/Mg-doped $TiO_2$, $SrTiO_3$, and NiO@GeSe core-shell nanorods can optimize energy level alignment, passivate defects, accelerate charge transport dynamics, and thereby enhance the open-circuit voltage (Voc).

Through comparative assessment of materials, preparation methods, and structural innovations, this review underscores that nanomaterials are central to overcoming current bottlenecks. The strategic integration of tailored nanomaterials into transport layers, photoactive absorbers, and electrode structures not only enhances power conversion efficiency but also improves device stability and scalability. These advances collectively highlight

nanomaterials as a key enabler for the transition of PSCs from laboratory research to practical photovoltaic technologies.

Table 4. Nanomaterials in electrodes

| Nanomaterial | Mechanism | Effect Size | Processability | Cost | Reference |
|---|---|---|---|---|---|
| Carbon Nanotubes (CNTs)/Graphene Nanosheets | Enhance flexibility; high electron mobility; moisture barrier | CNTs mobility = $2\times10^5$ $cm^2V^{-1}s^{-1}$; graphene enables ultrathin devices | CNTs easy to form films; graphene layer number hard to control | Medium | [77,80] |
| Oxide/Metal/Oxide (OMO) Structures (ITO/Ag/ITO, $SnO_2$/Ag/$SnO_2$) | Balance transparency, conductivity, and mechanical resilience | Transmittance >85 %; square resistance <10 Ω/sq | Layer-by-layer deposition (sputtering); precise thickness control required | Medium | [84,87] |
| Metallic Grids (Ag/Cu) | Reduce electrode resistance; enhance light transmittance | Optical-electrical trade-off optimized; semi-transparent PSC compatible | Photolithography/ printing process; grid pattern easy to customize | Low | [88] |
| Silver Nanowires (Ag NWs) | Provide flexible conductive channels; balance transparency/ conductivity | PCE comparable to ITO electrodes; bending stability >1000 cycles | One-step doctor-blade coating; composite films (Ag NWs-ZnO) processable | Medium | [89,95] |
| Copper Nanowires (Cu NWs) | Low-cost conductive network; flexible electrode construction | Transparency >80% for thin films; conductivity close to Ag NWs | Solution-processable; prone to oxidation during storage/processing | Low | [97] |

## Challenges and future directions

Device- and materials-level challenges for nanomaterial-enabled PSCs. Despite significant progress, nanomaterial-enabled perovskite solar cells (PSCs) still face several critical challenges that hinder large-scale commercialization. First, nanomaterial-perovskite interfaces are prone to degradation under prolonged illumination, elevated temperature, and humid environments, leading to progressive efficiency losses. Second, laboratory-scale nanomaterial synthesis is difficult to scale up, which results in poor batch-to-batch consistency and increased production costs. Third, lead-based perovskite systems raise environmental concerns, while some nanomaterials (such as Cu nanowires) suffer from limited oxidation resistance and insufficient compatibility with perovskite precursors. In addition, the synergistic

effects of multi-layer nanomaterial architectures and their long-term structure-performance relationships remain insufficiently understood. Finally, the reliance on high-quality nanomaterials (for example, Au nanoparticles or graphene) together with complex nanostructuring processes increases manufacturing cost and currently limits the competitiveness of PSCs relative to mature photovoltaic technologies.

Challenges in numerical modeling and predictive design. Although numerical modeling provides crucial theoretical guidance for perovskite solar cell (PSC) optimization, it still exhibits notable limitations arising from the required simplifications and idealized assumptions. Most models presuppose ideal nanostructures and neglect fabrication-induced defects such as surface roughness, impurities, and lattice mismatches. They typically operate under ideal environmental conditions, for example, constant temperature and dry atmosphere, without accounting for practical factors, including humidity, temperature fluctuations, and variable light intensity. Complex interfacial charge-transfer and recombination mechanisms are often oversimplified, and defect-induced non-radiative recombination is frequently ignored in plasmonic simulations, which can lead to overestimated light absorption. Many studies focus on local structural units, such as single nano-pyramids or individual nanowires, while overlooking macroscopic effects such as large-area array uniformity and interlayer contact resistance, thereby limiting the guidance that can be provided for large-scale fabrication. In addition, nanomaterial long-term aging, such as Cu nanoparticle oxidation or Ag nanowire migration, is commonly disregarded. Collectively, these limitations introduce non-negligible deviations between simulated and experimental results, lead to overestimation or underestimation of key device effects, and restrict the predictive capability of numerical models for the long-term stability of PSCs.

Future directions. To address the above challenges in nanomaterial-enabled PSCs, future research should prioritize the development of durable, multifunctional nanocomposites and ultrathin passivation layers that simultaneously enhance device stability and suppress non-radiative recombination. Efforts are also needed to optimize low-temperature, roll-to-roll compatible fabrication processes, in order to improve scalability and batch-to-batch consistency through precise control over nanomaterial morphology, distribution, and interfaces. Replacing noble metals with earth-abundant, environmentally benign alternatives and designing lead-free hybrid perovskite-nanomaterial systems will be essential to reduce both cost and toxicity. In parallel, the synergistic interactions among nanomaterials in different layers should be systematically investigated, and robust long-term reliability evaluation protocols should be established. It is further desirable to explore multifunctional nanomaterials that integrate light-harvesting enhancement, charge-transport promotion, and defect passivation, and to implement them in tandem architectures to broaden the spectral response and push device efficiencies toward their practical limits. Overall, the rational design of nanomaterials for PSCs requires a holistic framework that balances these intertwined effects, rather than optimizing a single parameter in isolation, and should combine materials chemistry, interface engineering, and optical/electrical modeling to identify truly synergistic nanostructures.

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