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Review

The Use of Core-Shell Nanoparticles in Photovoltaics

Alexander Quandt [1,2,3,*], Daniel Wamwangi [1,4] and Sandile Kumalo [1]

[1] School of Physics, University of the Witwatersrand, Private Bag 3, Wits 2050, South Africa; daniel.wamwangi@wits.ac.za (D.W.)
[2] Istituto di Fotonica e Nanotecnologie-Consiglio Nazionale delle Ricerche (IFN-CNR), Characterization and Development of Materials for Photonics and Optoelectronics (CSMFO) Laboratory and Fondazione Bruno Kessler (FBK) Photonics Unit, Via Alla Cascata 56/C, 38123 Povo, TN, Italy
[3] Photonics Laboratory of Angers LPhiA, SFR MATRIX, University of Angers, 2 Bd Lavoisier, 49045 Angers, France
[4] Materials Physics Research Institute, University of the Witwatersrand, Private Bag 3, Wits 2050, South Africa
* Correspondence: alex.quandt@wits.ac.za

Abstract: The field of photovoltaics (PV) continually seeks innovative materials solutions to enhance the efficiency and the stability of their standard devices. Core-shell nanoparticles have emerged as a promising new technology with unique structural attributes and widely tunable properties. This paper reviews the use of plasmonic core-shell nanoparticles in PV applications through various experimental validations. We describe advancements in the design and in the control over the properties of core-shell nanoparticles and highlight their integration into various solar cells, based on their ability to finely tune optical, electronic, and chemical properties. We also discuss experimental results for organic, perovskite, and dye-sensitized solar cells, where core-shell nanoparticles have been successfully deployed. Additionally, we identify gaps in the current research, such as the need for scalable synthesis methods and long-term stability assessments, and we will point out promising new developments at the frontier of that field.

Keywords: photovoltaics; plasmonic; core-shell nanoparticles

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1. Introduction

The global energy transition has highlighted the need for efficient, sustainable, and scalable renewable energy technologies [1]. Among these, photovoltaic (PV) systems, which convert sunlight directly into electricity, play a key role [2–4]. However, the cost of solar energy is not competitive with existing energy solutions. This is in part attributed to the costly fabrication of Si-based devices and the associated stringent material requirements. Therefore, the transition from bulk single crystal Si photoactive layers to thin films-based solar cells requires some practical trade-offs of the photo-absorption in the visible and near infra-red region. Even though there have been significant advancements in photoactive layer developments, challenges related to material properties, device physics, and operational limits continue to hinder their widespread adoption [5–8].

To address these challenges, researchers are exploring a range of strategies to improve light absorption, enhance the generation of excitons (bound electron-hole pairs) in materials where Coulombic attraction is significant, promote efficient exciton dissociation into free charge carriers, and facilitate the transport of these carriers in diverse photovoltaic devices. One promising approach is the incorporation of nanomaterials, particularly plasmonic nanoparticles (NPs), which exhibit tunable localized surface plasmon resonance (LSPR).

This unique optical phenomenon enables the manipulation of light at the nanoscale, enhancing the optoelectronic properties of the active layer and thereby the efficiency of PV devices [9–14].

An important advancement in this field is the development of core-shell NPs. These nanoparticles consist of a plasmonic core (typically a noble metal) surrounded by a dielectric shell. There is a lot of flexibility in the design of these nanoparticles, which allows for tunable optical properties, exciton generation, and improved charge transport, making them attractive for PV applications [15–17]. Another variant of the core-shell structure is the bimetallic core-shell nanoparticle, which consists of a metallic core and a different metallic shell. These core-shell structures have attracted extensive research interest due to their high photon trapping abilities and greater flexibility in modulating the plasmonic resonances through shell thickness variations [18,19].

This review paper is structured as follows: In the following section, we discuss the design principles and the most useful properties of plasmonic core-shell NPs, with a focus on their optical and electronic properties. Next, we examine their integration into various types of solar cells, including organic, perovskite, dye-sensitized, and inorganic PV devices. We also address the challenges associated with deploying these NPs in commercial applications and propose potential solutions. Finally, we conclude with a discussion on future research directions in this rapidly evolving field.

2. Design and Properties of Core-Shell Nanoparticles

2.1. Introduction to Core-Shell Nanoparticles

Nanotechnology has revolutionized material science by enabling the careful design and development of complex material systems through the control of atomic configurations, dimensionality, and patterning. As a result, research on nanostructures of varying geometry and aspect ratios, such as core-shell nanoparticles, has gained traction due to their unique, tunable properties and broad applicability in fields such as energy, electronics, and biomedicine. Core-shell nanoparticles consist of a core material surrounded by a shell that modifies their optical, electrical, and chemical characteristics [20]. By adjusting the core diameter and shell thickness, the LSPR characteristics, such as resonance wavelength, intensity, and field enhancement, can be precisely tuned, enabling more effective control of light–matter interactions compared to homogeneous nanoparticles. Additionally, core-shell architectures provide an inherent advantage in passivating surface defects, a challenge often encountered in homogeneous nanoparticles [21–23].

The unique properties of core-shell nanoparticles arise from the interaction between the core and the shell, which modifies light–matter interactions, resonance phenomena, and charge transport [24]. By designing the core-shell interface, researchers can achieve enhanced light absorption, reduced recombination losses, and improved charge transport. These features are particularly relevant for advanced optoelectronic applications, including solar cells.

2.2. Synthesis and Characterisation

2.2.1. Synthesis Methods

The formation of core-shell nanoparticles typically relies on multi-step synthesis routes, each offering unique advantages in controlling particle composition, morphology, and functionality. Common strategies include chemical reduction, seed-mediated growth, thermal decomposition, laser ablation, and templating techniques. These methods are often sequentially to achieve the desired core-shell architecture.

Chemical reduction is frequently used as an initial step to generate metallic nanoparticle seeds. It involves reducing metal precursors in the presence of stabilizing agents and

allows good control over particle size and dispersion. While not sufficient for core-shell formation on its own, this step serves as the foundation for subsequent shell growth [25–30].

Building upon this, seed-mediated growth involves depositing a secondary material around preformed cores. This approach enables precise control over the shell thickness, composition, and overall particle geometry, making it particularly suitable for tuning optical and electronic properties [31–33].

Thermal decomposition, involving the breakdown of organometallic or inorganic precursors at elevated temperatures, produces uniform nanoparticles with high crystallinity. When applied in sequence, the shell precursor decomposes after core formation, and this method can be adapted for core-shell synthesis. It is especially valued for its scalability and reproducibility when integrated into multi-step protocols [34–37].

Pulsed laser ablation in liquids (PLAL) is a clean and versatile technique for synthesizing core-shell nanostructures. It involves focusing a high-energy femtosecond laser on a solid target submerged in liquid, generating a plasma plume that condenses into nanoparticles. Core-shell architectures can be achieved by ablating layered targets or using sequential ablation steps [38]. A recent study demonstrated the fabrication of Ti@W core-shell photocatalytic films using PLAL, where tungsten was deposited onto titanium substrates without the use of surfactants [39]. The resulting films exhibited superhydrophilic surfaces (contact angle < 5°) and enhanced visible-light photocatalytic activity, making them effective for self-cleaning applications.

Beyond discrete particle synthesis, creating ordered arrays of core-shell nanoparticles is critical for applications such as photonic crystals and sensors. Techniques like block copolymer lithography, often coupled with controlled shell growth, provide spatial patterning and uniformity over large areas. This method is particularly advantageous in device fabrication, where structural regularity is essential [40–42].

2.2.2. Characterization Techniques

The characterization of core-shell nanoparticles is crucial for understanding the relationship between their structural and optical properties, which are key to their performance in various applications. Several advanced techniques are used for this purpose, providing complementary insights into the morphology, composition, and optical behavior of these structures.

UV-Vis spectroscopy measurements are commonly employed to study optical absorption, particularly localized surface plasmon resonance (LSPR) and other optical properties when embedded in the photoactive or buffer layers. This method provides insights into how particle size, shape, and composition affect LSPR excitations and other modes [43–45]. The combination of UV-Vis spectroscopy with structural analysis helps establish correlations between the optical and structural properties of the nanoparticles.

Photoluminescence (PL) spectroscopy is a powerful tool for probing the electronic and optical properties of core-shell nanoparticles, particularly in the context of photovoltaic applications [46–48]. PL measurements, as shown in the spectra in Figure 1a, provide insights into exciton dynamics, recombination pathways, and energy transfer efficiency within the nanostructures. These properties are strongly influenced by the core-shell configuration, which can affect light absorption, emission peak positions and widths, and the spatial distribution of charge carriers [49–51]. For instance, spectral shifts observed in PL spectra can indicate changes in band alignment or enhanced exciton separation efficiency due to the presence of a shell layer [52–55]. Such analysis helps to distinguish between radiative recombination, non-radiative losses, and energy transfer mechanisms. Understanding and controlling these processes is essential for optimizing the design of core-

shell nanoparticles to improve charge extraction and overall energy conversion efficiency in photovoltaic devices.

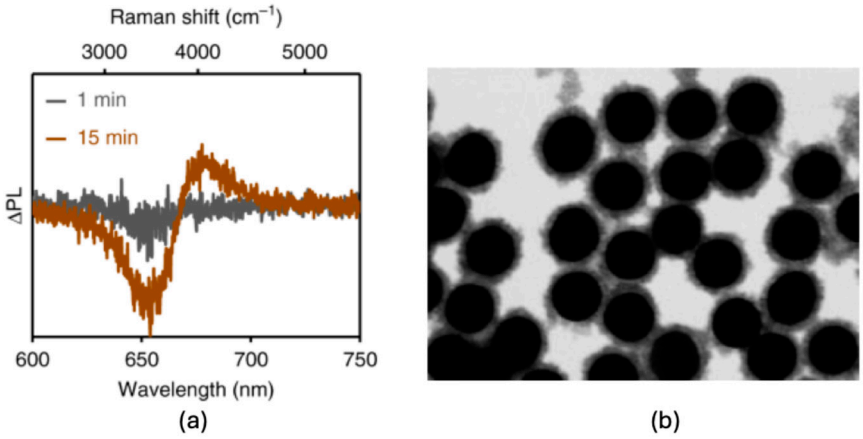

Figure 1. (**a**) Photoluminescence (ΔPL) spectra of photothermally grown Au@CeO_2 core@shell nanorod at t = 1 min (gray) and t = 15 min (brown). (**b**) Representative transmission electron microscopy (TEM) image showcasing the morphology of Au@CeO_2 core-shell NPs. Reproduced with permission from Ref. [55]. Copyright 2020, Springer Nature.

Transmission electron microscopy (TEM) is a standard method for structural analysis, offering high-resolution images of nanoparticle morphology. This technique, when applied to core-shell nanostructures, yields morphological information as shown in Figure 1b to enable precise correlation of optoelectronic properties with the geometrical measurements of core size, shell thickness, particle shape, and chemical composition. It also facilitates statistical analysis of particle size and shape distributions, which are critical for ensuring uniformity in nanoparticle synthesis and understanding their influence on performance [56–59].

2.3. Properties of Core-Shell Nanoparticles

2.3.1. Optical Properties

The optical absorption and scattering characteristics of core-shell nanoparticles are influenced by the aspect ratio, dielectric shell thickness, and core size. Adjusting the shell thickness (t) relative to the core radius (R_{core}) produces distinct optical effects. For thin shells (t < R_{core}), plasmonic behaviour is primarily dominated by the core, with the dielectric shell acting mainly as a spacer that isolates the core from environmental interactions, enhancing scattering cross-sections but offering limited influence over the plasmon resonance position. When the shell thickness approaches the core radius (t ≈ R_{core}), strong coupling between core and shell materials occurs, altering both absorption and scattering behavior and providing a balanced enhancement of the optical response. For thick shells (t > R_{core}), the dielectric shell significantly modifies the surrounding electric field distribution, allowing fine-tuning of the plasmon resonance to align with specific wavelengths within the solar spectrum [60].

Core-shell nanoparticles offer significant advantages in PV applications. Their structural versatility allows for optimization of key processes, including light absorption, exciton generation, and charge transport. By surrounding the core with a dielectric shell, the nanoparticle's interaction with light can be finely controlled, enhancing the overall photovoltaic process [61–64]. Commonly used dielectric materials for shells include silica (SiO_2), titanium dioxide (TiO_2), zinc oxide (ZnO), and alumina (Al_2O_3). These materials not only passivate the core surface but also improve light scattering and charge transport, contributing to enhanced PV device performance [65–67].

In addition, rare-earth oxides, such as cerium oxide (CeO_2), yttrium oxide (Y_2O_3), and lanthanum oxide (La_2O_3), are emerging as promising shell materials. These oxides exhibit dynamic and active optical properties, making them ideal for advanced PV applications [68]. Their ability to facilitate down-conversion and up-conversion processes is particularly noteworthy. These processes involve converting high-energy photons into multiple low-energy photons or vice versa, effectively broadening the absorption spectrum and improving the overall efficiency of photovoltaic devices. Such advancements highlight the potential of core-shell nanoparticles to drive innovation and enhance performance in next-generation solar technologies [69–71].

2.3.2. Electrical and Chemical Properties

The diverse configurations of core-shell nanoparticles are shown in Figure 2. These architectures offer specific advantages depending on the target application. For instance, yolk–shell structures (Figure 2a) provide void space for energy storage or catalytic activity, while multilayered shells (Figure 2c) allow spectral tuning across multiple optical regimes. Surface-functionalized systems (Figure 2f) are crucial for biological or chemical sensing due to their customizable interfaces. The dielectric materials used in these NPs are typically insulators with low electrical conductivity but high polarizability suited for screening the electric field around the NP and to enhance plasmonic effects [72]. The quality of the interface between the metal and dielectric is critical, as smooth, well-defined interfaces minimize light scattering losses and allow for more efficient plasmonic resonance [73]. Some common dielectric materials include the following:

(i) **Silica (SiO_2):** Silica is chemically inert and transparent across the solar spectrum, making it ideal for encapsulating plasmonic cores like Au or Ag. The silica shell protects the core from oxidation and aggregation while fine-tuning the particle's SPR [74].

(ii) **Titanium Dioxide (TiO_2):** TiO_2 has a high refractive index, which enhances light scattering in core-shell nanoparticles. As a wide-bandgap semiconductor, it also facilitates electron transport in photovoltaic applications, especially in its anatase phase. Moreover, varying the shell thickness of the TiO_2 layer enables fine-tuning of the plasmon resonance wavelength and optical response, providing broader design flexibility compared to many other dielectric materials [75–77].

(iii) **Zinc Oxide (ZnO):** ZnO offers excellent electron mobility and is used as a shell material to enhance electron transport and light absorption in PV devices [78–80].

(iv) **Alumina (Al_2O_3):** Alumina is chemically resistant and acts as an insulating shell that prevents recombination, enhancing charge transport [81].

(v) **Polymeric Shells:** Flexible, organic-compatible polymers like polystyrene or polyvinyl alcohol are used in applications where dispersion within organic matrices is needed [82,83].

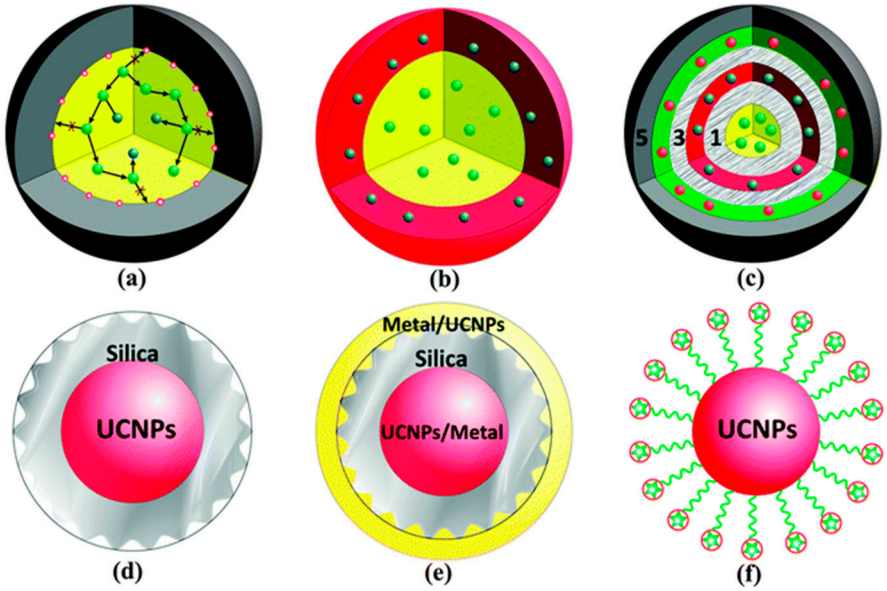

Figure 2. Schematic representations of different core–shell nanoparticle configurations: (**a**) Yolk–shell structures with a movable core inside a hollow shell, allowing for enhanced surface area and dynamic core–shell interactions; (**b**) Multicomponent core–shell with distinct compartmentalized regions for multifunctional applications; (**c**) Multilayered core–shell (layer-by-layer) with alternating materials offering tunable optical and electronic properties; (**d**) Classic core–shell with an upconversion nanoparticle (UCNP) core and silica shell for optical protection and surface passivation; (**e**) Composite core–shell with embedded metal/UCNP structures within silica for plasmon-enhanced upconversion; (**f**) Surface-functionalized UCNPs for targeted delivery or improved solubility via organic ligands or polymers. Reproduced with permission from Ref. [64]. Copyright 2015, The Royal Society of Chemistry.

3. Applications of Core-Shell Nanoparticles in Photovoltaics

3.1. Organic Solar Cells

Organic solar cells remain a cost effective and versatile PV technology that has gained rapid research attention [84–88]. Despite their enormous potential, they are limited by the short exciton diffusion length, which constrains carrier extraction. These diffusion lengths restrict the thickness of the photoactive layer to hundreds of nm, thereby limiting the photo-absorption and power conversion efficiency (PCE) in general [89,90]. A strategy to circumvent this limitation involves the use of plasmonic nanostructures to efficiently boost the light harvesting by the photoactive layer. Therefore, various core-shell NPs have been widely integrated into organic solar cells to enhance light absorption, exciton generation, and charge transport [91–93]. In the following sections, we present examples of enhanced performance in organic solar cells achieved by incorporating core-shell structures into the device architecture.

3.1.1. Augmentation of Active Layers

A promising strategy for enhancing photovoltaic performance involves embedding core-shell nanoparticles directly into the active layer of solar cells, as illustrated in Figure 3a. This approach has demonstrated improved light absorption in materials such as P3HT- or PTB7-based blends [94,95]. Embedding core-shell nanoparticles within the active layer significantly enhances light harvesting by amplifying localized electromagnetic fields [96]. This enhancement leads to improved absorption and exciton generation, enabling more efficient energy conversion. Studies by Zhang et al. have shown that incorporating core-shell nanoparticles into P3HT- or PTB7-based blends boosts the absorption of incident

light, facilitating greater exciton generation and contributing to improved overall device performance [97–99].

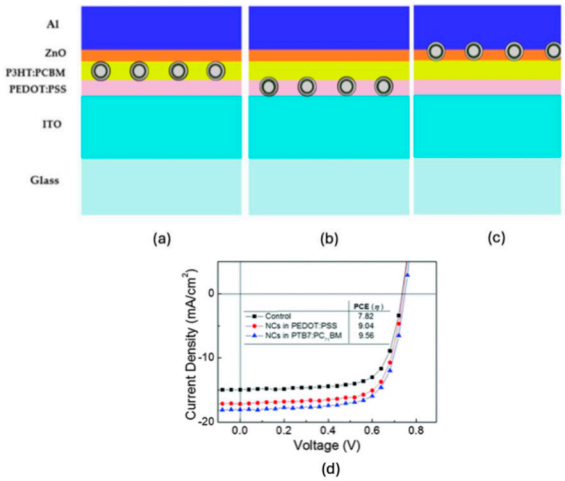

Figure 3. A schematic depicting the embedding of core-shell nanoparticles in (**a**) the active layer, (**b**) the hole transport layer, and (**c**) the electron transport layer of an organic solar cell. (**d**) Shows the J-V characteristics of devices with core-shell nanoparticles embedded in these layers. Reproduced with permission from Refs. [90,93]. Copyright 2016, The Royal Society of Chemistry and Copyright 2023, MDPI Micromachines.

3.1.2. Augmentation of Buffer Layers

Another strategy consists of incorporating core-shell NPs into the buffer layers through the near-field effect, such as the hole transport layer (HTL) or electron transport layer (ETL), shown in Figure 3b,c. The incorporation may involve either regular arrays of core-shell NPs or random embedding within these layers. For large core-shell structures, typically with core diameters of 100 nm or more, light trapping due to strong scattering effects dominate over absorption. These larger NPs can act as efficient scattering centers, extending the optical path length within the device and thus promoting greater light absorption in the active layer [100,101].

In contrast, smaller core-shell NPs with core diameters below 50 nm are more effective at generating localized near-field effects, which can increase exciton generation at the active layer interface. The proximity of these small NPs to the organic materials amplifies the near-field enhancement, benefiting charge separation and improving carrier extraction [102–105].

In the case of regular arrays, the periodicity and spacing of the nanostructures determine the nature of the LSPR excitation, and broadband multiple absorption peaks are typically observed. Arrays of core-shell NPs can also serve as diffractive elements, further enhancing light trapping within the active layer and ultimately increasing light-harvesting efficiency [106,107]. These configurations offer versatile pathways for selecting core-shell NPs tailored to enhance specific aspects of device performance as depicted in Figure 3d, depending on whether light trapping or near-field enhancement is prioritized.

3.2. Perovskite Solar Cells

While perovskite solar cells have demonstrated remarkable efficiency and stability in recent years, they still face certain limitations in their optical properties [108–110]. One major challenge is sub-optimal light absorption in the near-infrared (NIR) wavelengths, which reduces the overall photocurrent generation [111–116]. Additionally, the need to balance transparency with light harvesting in semitransparent perovskite solar cells restricts the thickness of the photoactive layer 150–300 nm, further limiting optical absorption and

device efficiency [117–121]. Core-shell nanoparticles are being implemented to address these issues through the following:

3.2.1. Light Harvesting Enhancement

The incorporation of core-shell nanoparticles into photovoltaic devices as depicted in Figure 4a,b, particularly semitransparent perovskite solar cells, offers substantial advantages for light harvesting [122–125]. Metallic cores, such as Au or Ag, enhance local electromagnetic fields through localized surface plasmon resonance (LSPR) effects, leading to improved light absorption. These metallic cores enable light to be concentrated into sub-wavelength regions, amplifying the local electromagnetic field and optimizing light harvesting. This results in enhanced photocurrent generation, as presented in Figure 4c, and an overall increase in PCE, as illustrated in Figure 4d [126,127].

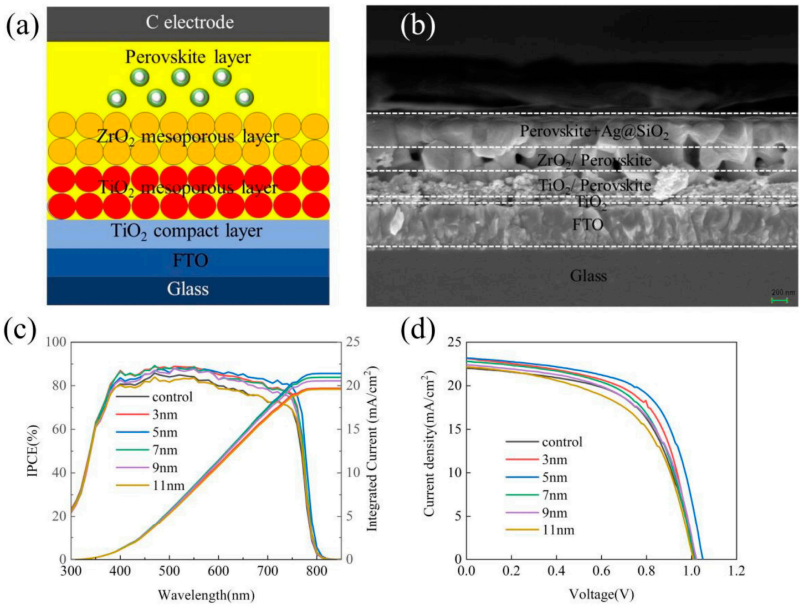

Figure 4. (**a**) Schematic representation of core-shell nanoparticles integrated into the perovskite layer. (**b**) SEM cross-sectional image of a perovskite solar cell (PSC) with core-shell NPs. (**c**) Incident photon to current conversion efficiency (IPCE) spectra of PSCs incorporating Ag@SiO_2 core-shell nanoparticles with varying shell thicknesses. (**d**) J-V characteristics of PSCs containing Ag@SiO_2 core-shell nanoparticles with different shell thicknesses. Reproduced with permission from Ref. [128]. Copyright 2020, MDPI Nanomaterials.

Despite these advantages, there are several practical challenges that must be addressed to fully realize the potential of core-shell NPs in perovskite solar cells. Issues such as material compatibility, achieving uniform dispersion of nanoparticles within the layers, and mitigating lead leaching from perovskite materials remain critical hurdles [129–131].

3.2.2. Stability Improvements

Dielectric shells provide critical stability enhancements for PSCs by shielding the sensitive perovskite layer from environmental stressors such as moisture, oxygen, and ultraviolet (UV) radiation. This protective barrier significantly enhances device longevity and operational stability, addressing one of the key challenges in perovskite solar cell technology [132–135].

Materials such as zinc oxide (ZnO) and titanium dioxide (TiO_2) are commonly employed as dielectric shells due to their dual functionality. These shells stabilize the perovskite layer while simultaneously improving electron mobility, facilitating efficient charge transport, and minimizing recombination losses. By integrating these dielectric shells,

PSCs achieve enhanced electron transport and greater resilience against environmental degradation [136–139].

The ability of dielectric shells to mitigate degradation mechanisms is pivotal in extending the lifespan and reliability of PSCs. Their multifunctional role as both a stabilizing and performance-enhancing component underscores their importance in advancing the practical deployment of perovskite-based photovoltaic devices.

3.3. Dye-Sensitized Solar Cells

Core-shell NPs enhance the performance of dye-sensitized solar cells (DSSCs) by improving light absorption, electron injection, and transport and minimising recombination. Embedding these NPs in the photoanode as illustrated in Figure 5a,b or adding these core-shell nanoparticles (Figure 5c) to the electrolyte both increase the optical path length. They also enhance light scattering, which increases photon absorption [140]. Additionally, dielectric shells such as ZnO or SiO_2 improve electron transport, and they minimize recombination, leading to improved overall device performance, as shown in Figure 5d,e [141,142].

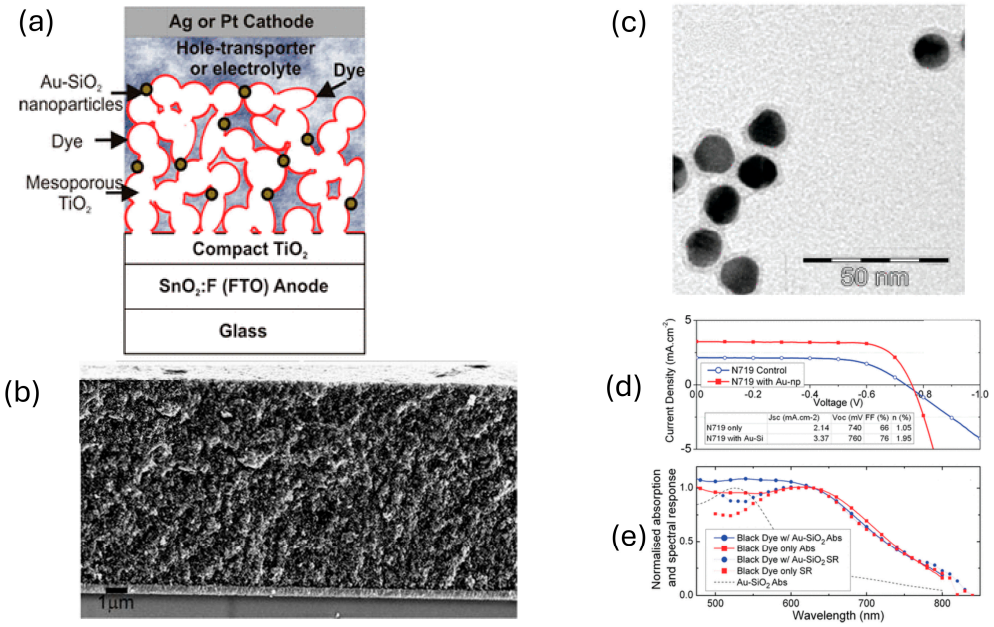

Figure 5. (**a**) Conceptual illustration of Au@SiO_2 core–shell nanoparticles embedded within the electrolyte of DSSCs, demonstrating their function in enhancing light absorption and facilitating charge transport. (**b**) Cross-sectional SEM image of a mesoporous TiO_2 photoanode incorporating Au@SiO_2 nanoparticles. (**c**) High-resolution depiction of core–shell nanoparticles featuring ~15 nm gold cores encapsulated by ~3 nm silica shells. (**d**) Current–voltage (J-V) characteristics of DSSCs showing the impact of Au@SiO_2 nanoparticle incorporation on device performance. (**e**) Comparison of normalized absorption and IPCE spectra for DSSCs with and without Au@SiO_2 integration. Reproduced with permission from Ref. [143]. Copyright 2010, American Chemical Society.

Energy level alignment is another important benefit, where the presence of core-shell NPs ensures more efficient electron transfer between the dye, the semiconductor, and the electrolyte [144]. DSSCs with integrated core-shell NPs have shown clear improvements in photocurrent and in PCE [145–149], where reductions in recombination losses, improved light harvesting, and better electron injections have led to PCE increases of 10–30%, thus contributing to much more efficient DSSCs [150–152].

3.4. Inorganic Solar Cells

The integration of core-shell NPs into inorganic solar cells has proven to be a promising approach for enhancing device efficiency. These nanoparticles play a critical role in improving light absorption, reducing reflection losses, and managing thermal effects in silicon-based and thin-film solar cells [153–155].

Enhanced Light Scattering and Trapping

Core-shell nanoparticles are instrumental in enhancing light absorption within silicon-based solar cells through effective light scattering and trapping mechanisms as demonstrated in Figure 6a,b. The dielectric shells of these nanoparticles scatter incoming light, increasing its optical path length within the active layer, which enhances photocurrent generation. This mechanism is particularly advantageous in reducing reflection losses, thereby allowing more light to be absorbed by the semiconductor material [156–158].

In thin-film photovoltaic devices, such as cadmium telluride (CdTe) and copper indium gallium selenide (CIGS) solar cells, core-shell nanoparticles facilitate improved light absorption in thinner active layers. By doing so, they enhance device efficiency without compromising charge transport properties [159,160]. Furthermore, core-shell nanoparticles can serve as anti-reflective coatings, decreasing surface reflectivity and maximizing light transmission into the active layer, thus boosting the overall efficiency of silicon solar cells [161].

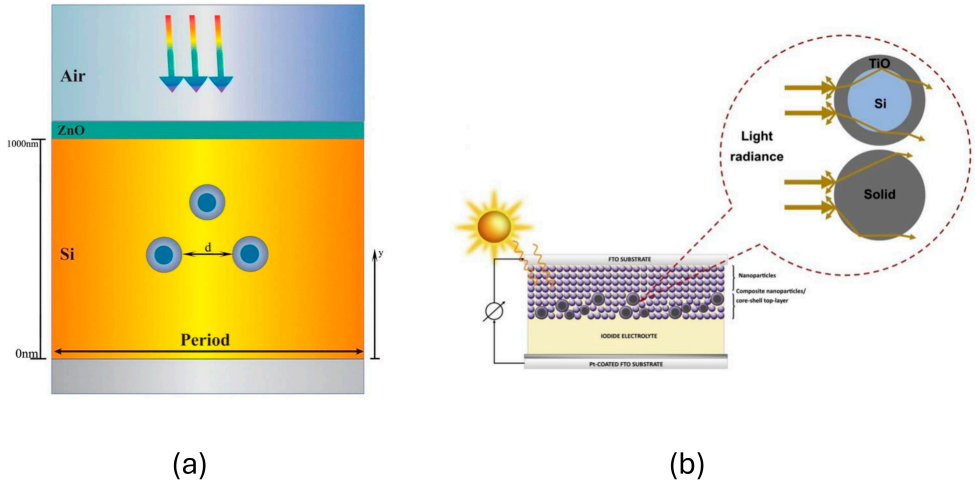

Figure 6. (**a**) Schematic representation of a silicon solar cell incorporating core-shell nanoparticles. (**b**) Illustration of incident light interaction with SiO_2-TiO_2 core-shell structures compared to solid sphere structures, highlighting their role in light transmission and scattering. Reproduced with permission from Refs. [162,163]. Copyright 2019, Springer and Copyright 2019, Elsevier.

4. Challenges and Future Directions

4.1. Current Limitations

Despite their great potential outlined in this review, core-shell NPs face several challenges that must be addressed before their widespread adoption in photovoltaic (PV) technologies. These challenges include scalability issues, high manufacturing costs, limited plasmonic resonance lifetimes, and material stability [164,165]. Current synthesis methods, such as chemical reduction and seed-mediated growth, are costly and lack precise control over the general patterning and regularity of NP arrays. This lack of control compromises reproducibility and scalability for large-area production, which is critical for industrial applications [166].

A significant issue is the difficulty in patterning regular arrays of core-shell NPs for broadband optical absorption [167]. While conventional lithographic methods, such as electron-beam lithography and femtosecond laser processing, offer precise patterning, they remain costly, requiring specialized facilities, and hence are not scalable for large-area devices or modules [168,169]. Soft lithography techniques, including microcontact printing and nanoimprint lithography, provide a cost-effective and scalable alternative for large-area nanopatterning, making them promising for photovoltaic applications [170,171]. Block copolymer self-assembly has also emerged as a viable bottom-up approach for fabricating periodic nanostructures, offering tunability and large-area scalability, though challenges in defect control and domain alignment remain [172]. Additionally, advanced patterning methods used in OLED display manufacturing, such as inkjet printing and nanoimprint lithography, could offer new avenues for integrating core-shell NP arrays into scalable photovoltaic technologies [173].

Additionally, while dielectric shells are effective in protecting NPs, the long-term stability of these interfaces under real-world conditions remains a concern. Environmental factors, such as exposure to moisture, UV light, and temperature fluctuations, can degrade the metal-dielectric interface, leading to performance loss over time [174,175].

Finally, environmental and toxicity concerns, especially with materials like Ag, Au, and Pb, pose sustainability challenges that need to be addressed for broader adoption [176]. Additionally, these elements are increasingly being scrutinized as critical materials in the energy transition, with potential supply constraints due to their competing demand in sectors such as electronics, catalysis, and battery storage [177]. For instance, Ag is extensively used in photovoltaic modules and electronic circuits [178–183], while Au is crucial for high-performance electronic components [184–186]. Lead, despite its established toxicity, remains in use in perovskite solar cells, raising concerns about long-term environmental impact and regulatory restrictions [187,188]. While this challenge is primarily associated with the perovskite material itself rather than the core-shell structure, the integration of core-shell nanostructures into perovskite solar cells (fourth-generation solar cells) presents opportunities for enhanced stability and performance. In this context, colloidal core-shell structures of halide perovskites could also be considered, as they offer multiphoton excitations, which can be advantageous for improving light-harvesting efficiency and carrier dynamics in next-generation photovoltaic devices [189]. Exploring alternative materials or recycling strategies will be essential for ensuring the sustainable deployment of core-shell NPs in PV applications.

4.2. Some Solutions

To address these challenges, targeted approaches are needed that provide direct solutions to the high cost and low scalability problems. Among them are the following:

1. Scalable Synthesis Techniques
    - **Advanced Synthesis Methods**: Continuous flow synthesis and template-assisted approaches offer better scalability and control over particle uniformity. For example, continuous flow systems provide consistent reaction conditions, improving monodispersity and reproducibility in large-scale production [190,191]. From the point of view of large-scale device fabrication, these methods are not yet industry-standard due to high initial setup costs and technical challenges in scaling to multi-ton production levels [192,193].
    - **Self-assembly with Directed Control**: Self-assembly techniques combined with external fields (electric or magnetic) can pattern nanoparticles into ordered arrays, improving optical performance while reducing fabrication costs. Large-scale

fabrication would require consistent control of nanoparticle positioning across large areas, which remains challenging and limits industrial adoption [194–197].

2. Integration into PV Devices
   - **Efficient Deposition Techniques**: Advanced deposition methods such as spin-coating, spray-coating, and inkjet printing of core-shell nanoparticles enable the incorporation of nanoparticles into large-area solar modules with little extra costs. For example, inkjet printing allows precise deposition of core-shell NPs into pre-designed patterns, ensuring optimal placement for enhancing light trapping and charge transport [198,199]. Despite all the progress made in recent years, there remain some serious obstacles for large-scale implementations, such as issues with nozzle clogging and ink formulation, which need to be addressed to improve reliability and throughput [200,201].
   - **Optimized Placement**: The placement of core-shell NPs within the active or transport layers of PV devices should be optimized based on the target performance metric, such as light absorption or charge extraction. While simulations provide valuable insights, translating these into practical fabrication methods requires standardized protocols and advanced computational design tools to address inconsistencies [202–204].
3. Improving Long-term Stability
   - **Robust Shell Materials**: Using advanced shell materials, such as alumina or zirconia, can enhance chemical and thermal stability. These materials resist environmental degradation and maintain performance under real-world conditions [205,206]. Large-scale fabrication would require the development of cost-effective and scalable methods for depositing such shells, as current approaches like atomic layer deposition are expensive and need further refinement [207].
   - **Encapsulation Techniques**: Encapsulation of the entire solar cell, using barrier films or coatings, can protect core-shell NPs from moisture, oxygen, and UV light, extending the operational lifetime of the device [208–210]. This additional step adds to manufacturing costs, which industries are reluctant to absorb unless significant performance gains are demonstrated [211].
4. Environmental Sustainability
   - **Non-toxic Materials**: Developing non-toxic alternatives to toxic materials (e.g., aluminium-based plasmonic nanoparticles instead of lead-based materials) is essential for sustainable adoption [212]. Despite all the progress made in developing these alternatives, achieving comparable optical properties with non-toxic materials remains a significant technical challenge [213–215].
   - **Lifecycle Assessment**: Comprehensive lifecycle assessments can help quantify the environmental impact of core-shell NPs, identifying areas where improvements can be made in material selection and processing [216,217]. These assessments are still in their infancy for many emerging nanoparticle technologies, hindering their industrial acceptance [218].
5. Advanced Material Design
   - **Bimetallic Core-Shell Structures:** Recent theoretical studies highlight the potential of bimetallic plasmonic core-shell structures with limited surface segregation. Combining metals with complementary properties (e.g., Au-Ag or Cu-Al) can result in core-shell NPs with tunable optical and electronic properties, tailored for specific PV applications. These designs leverage fundamental material properties, such as differences in cohesive energy and enthalpy of mixing, to achieve optimal

performance [219–222]. From the point of view of large-scale device fabrication, scalable and cost-effective synthesis of these structures remains an obstacle [223].

5. Conclusions

Core-shell nanoparticles represent a disruptive advancement in photovoltaic technologies, offering innovative solutions to major challenges like light absorption and charge transport. These NPs can be integrated into a wide range of PV technologies, including organic, perovskite, dye-sensitized, and inorganic solar cells, where they lead to significant improvements in efficiency and performance of these devices. A summary of typical experimental results is shown in Table 1. The data refer to standard photovoltaic devices and reflect the current benchmarks in the field.

Table 1. Summary of performance enhancements with plasmonic core-shell nanoparticles in photovoltaic devices.

Device	Type of Core-Shell Nanoparticles	Improvements in Efficiency	Reference
Organic Solar Cells	Ag@TiO_2	From 7.82% to 9.56%	[93]
Perovskite Solar Cells	Au@SiO_2	From 11.44% to 14.57%	[122]
Dye-Sensitized Solar Cells	Ag@PVP	From 7.04% to 7.9%	[224]

State-of-the-art research in this area continues to address the challenges of scalability, material compatibility, and environmental sustainability, where core-shell NPs hold the potential to drive the next generation of high-efficient, durable, and cost-effective solar cells. Mastering these new technologies will make solar energy more affordable and accessible worldwide, where advanced solar technologies have already become an essential part of a global transition towards sustainable and renewable energy production and consumption.

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