Design and optimization of polymer-based organic solar cells with enhanced photocurrent using plasmonic metal-metal core-shell nanoparticles

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Abstract

This study explores the influence of shell thickness on photocurrent density in polymer-based solar cells incorporating gold-silver (Au-Ag) and silver-gold (Ag-Au) metal-metal core-shell nanoparticles. Efficient light trapping and absorption in polymer solar cells remain a key challenge, necessitating innovative approaches to improve performance. Addressing this gap, the research investigates how variations in shell thickness impact the plasmonic enhancement of photocurrent density. Simulations reveal that increasing shell thickness initially boosts photocurrent density due to enhanced plasmonic effects but stabilizes or declines slightly beyond an optimal thickness. For example, at a cell thickness of 80 nm, photocurrent densities of 13.74 mA/cm², 16.62 mA/cm², and 19.3 mA/cm² were achieved for the reference cell (without nanoparticles), a cell with Ag nanoparticles, and a cell with Au-Ag nanoparticles, respectively. These results underscore the critical role of shell thickness and material composition in optimizing core-shell nanoparticles for maximizing solar cell efficiency, offering insights for advancing polymer-based photovoltaic technologies.

Keywords: Core-shell nanoparticles; organic solar cell; photocurrent; plasmonic nanoparticles; polymer solar cell.

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1. INTRODUCTION

Organic polymer solar cells have emerged as one of the leading technologies for solar energy conversion due to their unique features such as lightweight, mechanical flexibility, and the potential for large-scale production at low cost (Sorrentino et al., 2021; KV et al., 2024; Lewińska, 2024). However, the limited efficiency of these cells, especially in comparison to silicon-based solar cells and other first- and second-generation solar cells, remains a significant challenge (Chen et al., 2009; Kim et al., 2023). One of the most important factors affecting the performance of polymer solar cells is the insufficient light absorption in the active layer of these cells (Lee & Ebong 2017; Zhang et al., 2024). Therefore, numerous efforts have been made to improve light absorption efficiency and, consequently, increase the energy conversion efficiency of polymer solar cells. One promising solution in this field is the use of plasmonic nanoparticles (Omrani et al., 2021). Due to their ability to enhance the local electromagnetic field and induce surface plasmon resonance, plasmonic nanoparticles can significantly increase light absorption in polymer materials (Mandal, 2022; Zeng et al., 2023). This increased light absorption leads to enhanced electron-hole pair generation in the active layer, which directly impacts the final efficiency of the solar cell (Ike et al., 2022).

Among various nanoparticles, core-shell nanoparticles have attracted more attention due to their multidimensional capabilities in controlling and optimizing optical and electrical properties. In other words, plasmonic nanoparticles possess unique resonance characteristics that make them highly efficient in scattering and absorbing light over a broad spectral range. When these nanoparticles are strategically placed within or near the active layer of a solar cell, far-field enhancement effects can lead to increased light absorption across a wide range of wavelengths (Mousavifar et al., 2020).

The term "far-field effects" refers to the interaction of light with objects larger than the wavelength of the incident light. Plasmonic nanoparticles can scatter light in such a way that its path within the active layer of the solar cell is prolonged. This longer photon path increases the likelihood of absorption by the active layer, consequently improving the overall efficiency of the solar cell (Mousavifar et al., 2020). The optical properties of plasmonic nanoparticles can be tuned by controlling their size, shape, and composition. This allows researchers to design nanoparticles that resonate at specific wavelengths, enabling the spectral tuning of solar cells for better alignment with the solar spectrum.

Near-field effects arise from the interaction of light with sub-wavelength-scale structures, leading to highly concentrated electromagnetic fields near the surface of the plasmonic nanoparticles (Hägglund & Apell, 2012). This intense near-field enhancement can significantly increase light absorption by adjacent materials, such as the active layer of a solar cell. Near-field interactions between plasmonic nanoparticles and semiconductor excitons can lead to strong coupling phenomena, such as plasmon-exciton hybridization. This coupling can modify the energy landscape of excitons within the active layer of the solar cell, improving their absorption and dissociation efficiency.

By harnessing both far-field and near-field effects, researchers can design enhanced solar cells with better light absorption, higher charge generation, and overall improved efficiency. However, optimizing the spatial distribution, size, and shape of plasmonic nanoparticles, as well as integrating them with the solar cell structure, is essential to fully leverage these enhancements. Additionally, understanding the fundamental mechanisms governing far-field and near-field interactions is crucial for guiding the rational design of next-generation plasmonic solar cells. Core-shell nanoparticles can be designed in various configurations, such as metal-metal structures. Each of these configurations possesses unique properties that can differently impact the final performance of the solar cell. For

example, in metal-metal configurations, the metallic shell can contribute to improved light absorption by creating stronger plasmonic resonance. Thus, selecting the most suitable configuration for core-shell nanoparticles is of particular importance and requires a careful evaluation and comparison of these configurations' performance.

1.1. Purpose of study

In this study, a comprehensive examination and comparison of metal-metal configurations in plasmonic core-shell nanoparticles are conducted to evaluate the effect of each of these configurations on the efficiency of organic polymer solar cells with high optical current. The primary goal of this research is to provide optimization strategies for the design of polymer solar cells using these nanoparticles to achieve higher solar energy conversion efficiency. The results of this research could play a significant role in developing a new generation of highly efficient polymer solar cells, paving the way for broader utilization of renewable energy and achieving environmental goals.

2. METHOD AND MATERIALS

2.1. Simulation

This study provides a comprehensive analysis and comparison of metal-metal configurations in plasmonic core-shell nanoparticles to evaluate the impact of each configuration on the efficiency of polymer-based organic solar cells with enhanced photocurrent. The main goal of this research is to offer optimization strategies for the design of polymer solar cells using these nanoparticles to achieve higher efficiency in solar energy conversion. The results of this study can play a significant role in developing a new generation of high-efficiency polymer solar cells, paving the way for broader adoption of renewable energy and achieving environmental sustainability goals. Figure 1 illustrates the structural and compositional details of a polymer solar cell equipped with plasmonic core-shell nanoparticles. It presents a two-dimensional cross-section of the polymer solar cell, highlighting key components such as the bottom electrode, the active layer embedded with core-shell nanoparticles, and the hole transport layer. These layers work together to efficiently convert solar energy into electrical energy. The figure also depicts the different types of core-shell nanoparticles used in this study, emphasizing the innovative design and potential improvements in efficiency that can be achieved by integrating plasmonic core-shell nanoparticles into polymer solar cells. Figure A shows the schematics of the proposed polymer solar cell with metal-metal plasmonic core-shell nanoparticles.

Figure 1 shows the structural and compositional details of the polymer solar cell equipped with core-shell plasmonic nanoparticles. This figure presents a two-dimensional cross-section of the polymer solar cell, highlighting key components such as the bottom electrode, the active layer with embedded core-shell nanoparticles, and the hole transport layer. These layers work together to effectively convert solar energy into electrical energy. Additionally, the figure illustrates the various types of core-shell nanoparticles used in this study, generally emphasizing the innovative design and potential efficiency improvements achieved through the integration of core-shell plasmonic nanoparticles in polymer solar cells.

Figure 1

The structure of the simulated organic solar cell and its performance enhancement using metal-metal nanoparticles
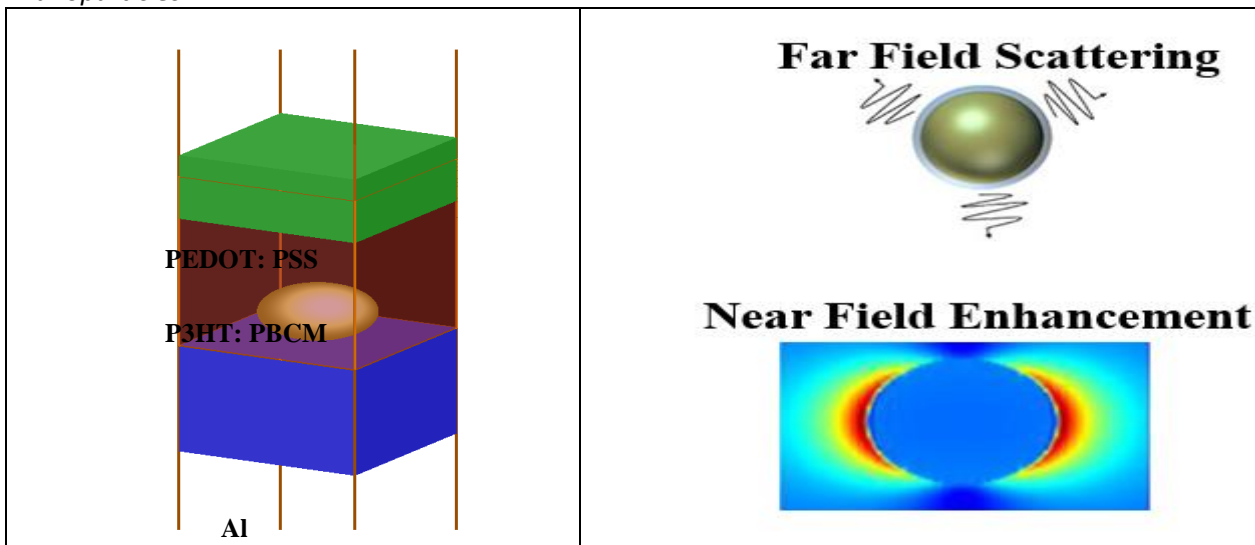
Maxwell's equations play a crucial role in modeling the behavior of plasmonic solar cells (Havryliuk et al., 2020). These equations, which govern the dynamics of electromagnetic fields, are essential for understanding how light interacts with materials at the nanoscale. In this process, Maxwell's equations are discretized in both space and time, and the distribution of electric and magnetic fields is calculated. By applying appropriate boundary conditions, such as Perfectly Matched Layer (PML) and periodic boundaries, the interaction of incident light with plasmonic nanoparticles and the surrounding environment is modeled. This simulation helps to understand the local electric field enhancements around the nanoparticles and their effect on increasing absorption within the active layer.

The absorption spectra obtained from these simulations are used to predict the photocurrent and the overall performance of the solar cell. Therefore, Maxwell's equations provide a fundamental framework for designing and optimizing plasmonic solar cells, enabling precise control and understanding of light-matter interactions at the nanoscale. The distribution of the electric field within the active layer under light irradiation is calculated, and the absorbed power is computed using Poynting's theorem and equation (1) (Heidarzadeh et al., 2016).

$$A(r, \lambda) = \frac{1}{2} \text{real} \left(\nabla \cdot \vec{P} \right) / P_{\text{in}} = \frac{1}{2} \frac{\omega \text{Im}(\epsilon(r, \lambda)) |E(r, \lambda)|^2}{P_{\text{in}}} \qquad (1)$$

Here, ω is the angular frequency, ϵ_0 is the permittivity of free space, ϵ is the dielectric constant, and E is the electric field. The short-circuit current is obtained by integrating the rate of electron-hole pair generation across the solar spectrum using equation (2).

$$J_{SC} = q \int_{\lambda_{\text{min}}}^{\lambda_{\text{max}}} \frac{A(\lambda) I(\lambda)}{\lambda} d\lambda \qquad (2)$$

Here, I(λ) is the intensity of the incident light, q is the electron charge, and A(λ) is the absorption spectrum. This method outlines a comprehensive approach to designing, simulating, and analyzing the performance of organic polymer solar cells enhanced with plasmonic core-shell nanoparticles. Through FDTD simulations and precise optical modeling, this study aims to optimize nanoparticle configurations to achieve maximum photovoltaic performance.

3. RESULTS

In this work, our goal is to improve the performance of organic polymer solar cells using plasmonic core-shell nanoparticles. Figure 2 shows the absorption spectra of polymer solar cells with different thicknesses, comparing cells combined with silver (Ag) and gold (Au) nanoparticles to cells without these nanoparticles. In panels (a) to (d) of this figure, the absorption spectra for various cell thicknesses, including 40 nm, 60 nm, 80 nm, and 100 nm, are shown respectively. Each panel illustrates how the presence of silver and gold nanoparticles affects the light absorption capabilities of the solar cells over a range of wavelengths. Specifically, the absorption spectra reveal an enhancement in light absorption between 600 to 800 nm for cells containing these plasmonic nanoparticles, highlighting their role in improving light absorption efficiency. The reason for this improvement lies in the plasmonic effect of the nanoparticles. The presence of plasmonic nanoparticles significantly increases absorption due to the interaction between the plasmonic effects generated by the nanoparticles and the thickness of the active layer. When these nanoparticles are exposed to light, the conduction electrons on the nanoparticle surface oscillate collectively at specific resonance frequencies. This oscillation leads to strong absorption and scattering of light, enhancing the local electromagnetic field around the nanoparticles. The local enhancement of the electromagnetic field near the nanoparticle surface increases the optical path length in the solar cell's active layer, causing more light to be absorbed by the polymer materials surrounding the nanoparticles, thus increasing the overall light absorption by the cell. Plasmonic nanoparticles can scatter incoming light, guiding it into the active layer and trapping it within the cell. This scattering effect increases the likelihood of light absorption by extending the optical path length through multiple internal reflections. This is especially beneficial for thin-film solar cells, where the optical path length is typically limited.

Figure 2

Comparison of the absorption spectra with and without Ag nanoparticles for a polymer cell with a cell thickness of (a) 40nm, (b) 60nm, (c) 80nm, and (d) 100nm.
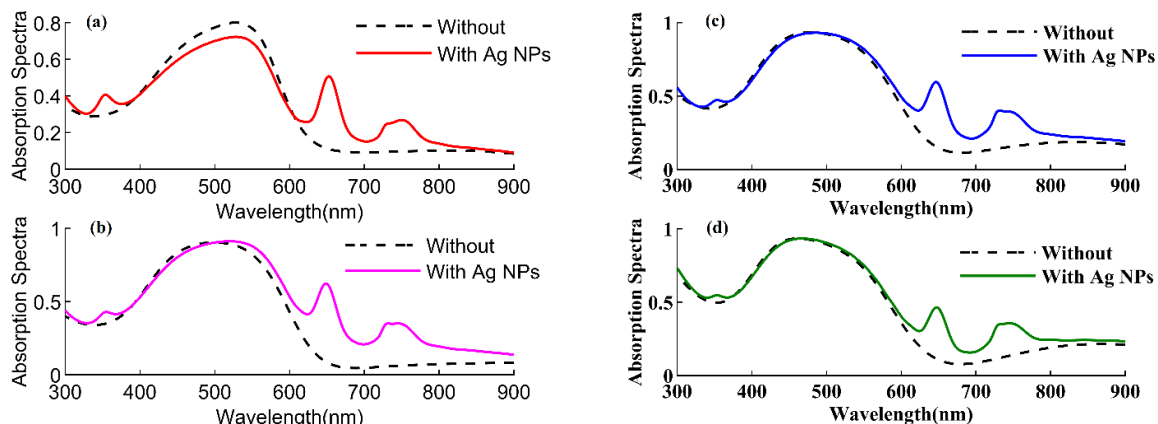
Figure 3 illustrates the photocurrent generated by polymer solar cells with and without plasmonic nanoparticles at different thicknesses (40 nm, 60 nm, 80 nm, and 100 nm). The results demonstrate the enhancement in photocurrent due to the presence of nanoparticles.

Figure 3

Comparison of the photocurrent of a cell with and without nanoparticles for cell thickness of 40nm, 60nm, 80nm, and 100nm.
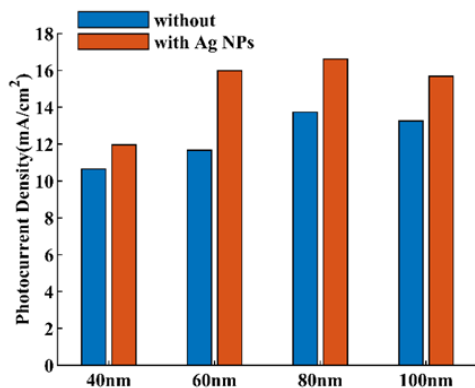
Figures 4 (a) to 4 (d) depict the photocurrent density as a function of shell thickness for solar cells with Au-Ag core-shell nanoparticles at different cell thicknesses of 40 nm, 60 nm, 80 nm, and 100 nm, respectively. For a cell with a thickness of 40 nm, the photocurrent density starts at around 12 mA/cm² without a shell and rapidly increases, reaching a maximum of about 14.5 mA/cm² at a shell thickness of 1 nm. After this point, the photocurrent density stabilizes in the range of 14 to 15 mA/cm² up to a shell thickness of 3 nm. These trends indicate that the enhancement of photocurrent density is highly dependent on the plasmonic properties of the core-shell nanoparticle configurations and the optimal shell thickness for maximum photocurrent density. Each configuration has its specific optimal thickness that maximizes performance, emphasizing the importance of material combination and structural design in solar cell efficiency.

Figure 4

Comparison of the photocurrent of a cell with and without nanoparticles for cell thickness of 40nm, 60nm, 80nm, and 100nm.
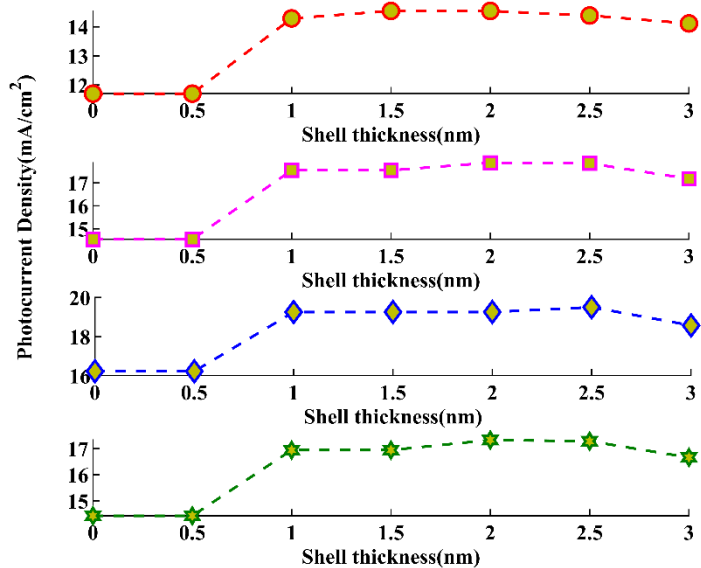
Figure 5 illustrates the electric field distribution for polymer solar cells incorporating plasmonic nanoparticles at two different wavelengths, comparing Ag nanoparticles with Au-Ag core-shell nanoparticles. In Figure (a), the electric field distribution around Ag nanoparticles at 700 nm shows strong localized near the nanoparticle surfaces, particularly at the edges, due to the plasmonic resonance effect, which significantly enhances light absorption in the active layer. In Figure (b), for Ag nanoparticles at 900 nm, the plasmonic effect is weaker, as Ag nanoparticles exhibit stronger resonance at shorter wavelengths. In contrast, figure (c) and (d) show the electric field distribution for Au-Ag core-shell nanoparticles at 700 nm and 900 nm, respectively. The plasmonic effect is more pronounced in the Au-Ag core-shell configuration, leading to stronger and more widespread electric field enhancements. This effect is particularly significant at 900 nm, where the combination of Au and Ag results in improved plasmonic coupling, enhancing light trapping and absorption across a broader wavelength range. This demonstrates the superior plasmonic performance of Au-Ag core-shell nanoparticles compared to pure Ag nanoparticles in maximizing light-harvesting efficiency.

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Figure 5

Electrical field distribution for a cell with Ag nanoparticles at wavelengths

(a)   (b)

(c)

(d)
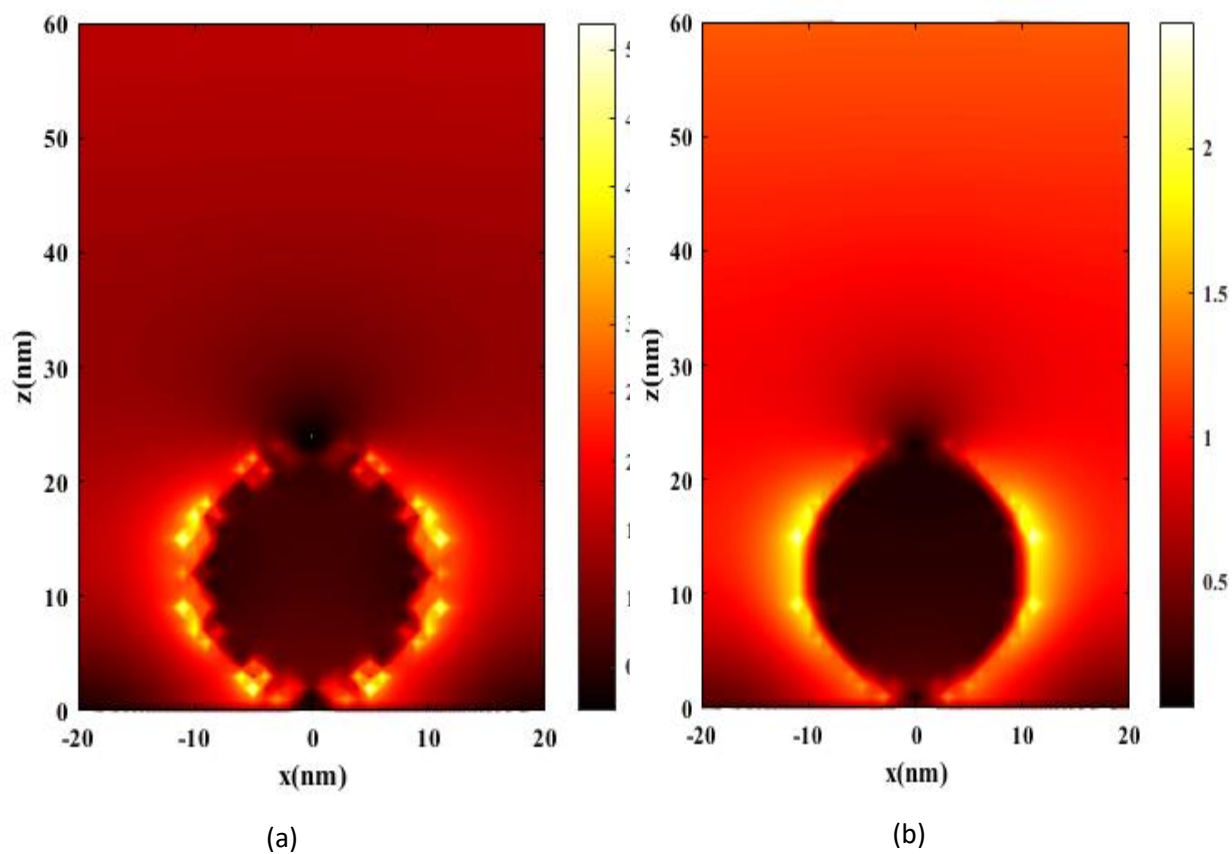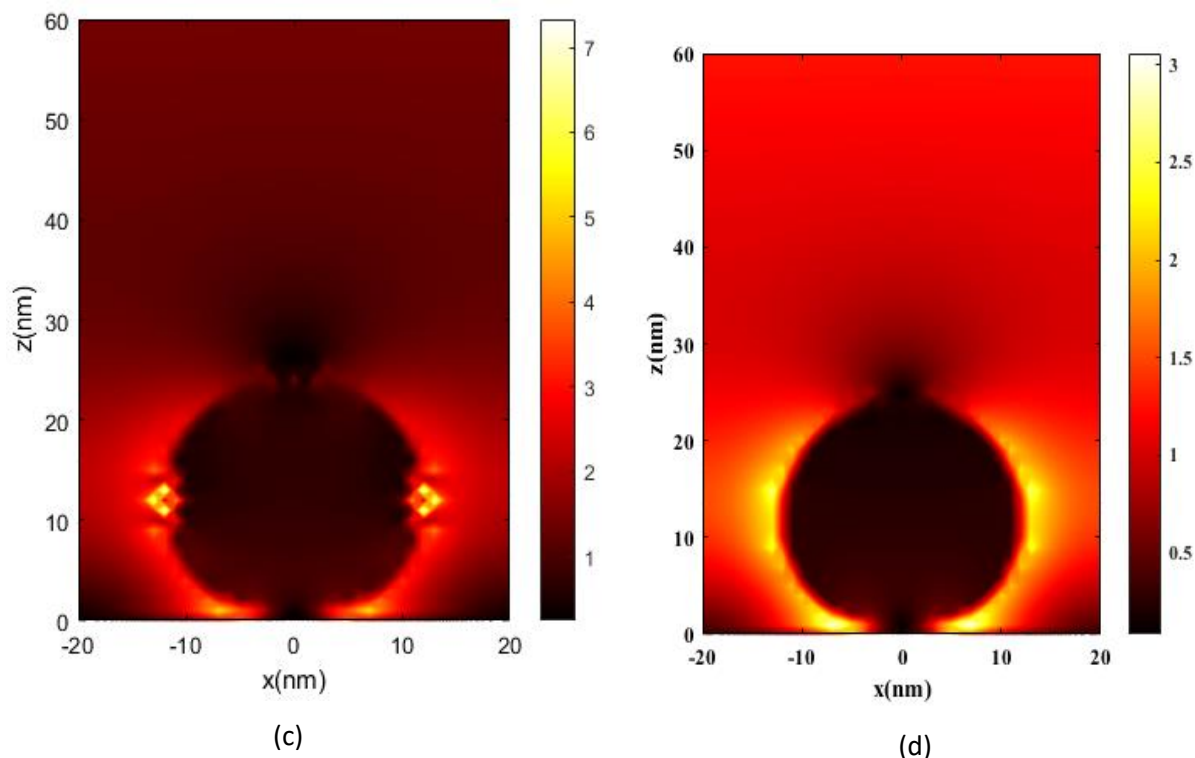
Note: (a) 700nm, and (b) 900nm, and Electrical field distribution for a cell with Au-Ag nanoparticles at wavelengths of (c) 700nm, and (d) 900nm.

4. DISCUSSION

In this work, the impact of the shell thickness of core-shell nanoparticles on the photocurrent density in polymer-based organic solar cells was investigated. The results indicate that as the shell thickness increases, the photocurrent density generally rises, reaching an optimal point before stabilizing or slightly decreasing. For example, for a cell thickness of 80 nm, the photocurrent density was measured in three different cases. In the cell without nanoparticles, the photocurrent density was 13.74 mA/cm². This value increased to 16.62 mA/cm² in the cell with Ag nanoparticles. The highest photocurrent density of 19.3 mA/cm² was observed in the cell containing Au-Ag nanoparticles.

The experimental and simulation results underscore the significant impact of plasmonic core-shell nanoparticles on the performance of polymer solar cells. The absorption spectra (Figure 2) demonstrate that the incorporation of Ag and Au-Ag nanoparticles enhances light absorption, particularly in the 600-800 nm wavelength range, across various cell thicknesses. This enhancement is attributed to the plasmonic effects of the nanoparticles, which include strong localized surface plasmon resonances (LSPRs) and effective light scattering, both of which amplify the electromagnetic field near the nanoparticles and extend the optical path length within the active layer. These effects are particularly beneficial in thin-film solar cells, where optical confinement is otherwise limited.

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The photocurrent data (Figure 3) further corroborates the role of plasmonic nanoparticles in boosting solar cell performance. The presence of nanoparticles consistently improves photocurrent across all examined thicknesses, with the magnitude of enhancement varying with the thickness and type of nanoparticle. This finding highlights the interplay between nanoparticle properties and active layer dimensions in achieving optimal light harvesting.

Figure 4 extends this analysis by examining the dependence of photocurrent density on shell thickness for Au-Ag core-shell nanoparticles. The results reveal a clear trend: photocurrent density increases with shell thickness up to an optimal value (1-3 nm) before stabilizing. This behavior reflects the balance between plasmonic enhancement and potential optical losses introduced by excessively thick shells, emphasizing the need for precise optimization of core-shell dimensions.

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Finally, Figure 5 illustrates the electric field distribution for Ag and Au-Ag nanoparticles, providing a detailed view of how plasmonic effects enhance light absorption. Compared to pure Ag nanoparticles, the Au-Ag core-shell configuration exhibits stronger and broader electric field enhancements, particularly at longer wavelengths. This superior performance is due to the synergistic plasmonic coupling between the gold core and silver shell, which enables more efficient light trapping across a wider spectral range. Overall, the Au-Ag configuration demonstrated better performance compared to Ag, which is attributed to the enhanced plasmonic effects in the Au-Ag combination, leading to improved light trapping and absorption.

5. CONCLUSION

This study demonstrates the effectiveness of plasmonic core-shell nanoparticles in enhancing the performance of polymer-based solar cells. Key findings include significant improvements in light absorption and photocurrent density due to the localized plasmonic resonance effects of Ag and Au-Ag nanoparticles. The results indicate that the optimal shell thickness for Au-Ag core-shell nanoparticles lies between 1 and 3 nm, beyond which performance stabilizes or slightly diminishes.

The superior plasmonic performance of Au-Ag core-shell nanoparticles compared to pure Ag nanoparticles is particularly noteworthy, as it extends the spectral range of light absorption and enhances light trapping efficiency. These findings underscore the importance of tailoring nanoparticle configurations and dimensions to maximize the efficiency of polymer solar cells.

By integrating plasmonic nanoparticles into thin-film solar cells, this work provides a pathway for advancing cost-effective and high-performance photovoltaic technologies. Future research should focus on experimental validation of the proposed configurations and exploring the scalability of such designs for commercial applications.

Conflict of interest: No potential conflict of interest was reported by the authors.

Ethical Approval: The study adheres to the ethical guidelines for conducting research.

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