

Improving light trapping of polymer solar cell via doping a new array of triple core-shell spherical nanoparticles utilizing realistic modeling



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ABSTRACT

The local surface plasmon resonance (LSPR) effects of metallic nanoparticles (such as light scattering and giant local field) in organic materials can improve the optical absorption capability of organic solar cells. This is especially important for polymer solar cells where the active layer thickness has been limited (< 150 nm) due to short electron-hole diffusion length. LSPR effects depend on the features of nanoparticle, such as shape and size. A cubic nanoparticle produces a stronger LSPR compared to other shapes and increased LSPR effect increases the light absorption. However, fabrication of the cubic nanoparticle is much more difficult compared to fabrication of spherical ones. This study aims to increase LSPR effects of spherical nanoparticles and we propose the $\text{SiO}_2/\text{Au}/\text{SiO}_2$ new structure for them. Our simulation results demonstrate increase in power absorption and short circuit current of $\sim 103\%$ and $\sim 118\%$, respectively, with square array of $\text{SiO}_2/\text{Au}/\text{SiO}_2$ nanoparticles with central nanoparticle inserted in thin active layer compared to the structure without nanoparticles. Subsequently, we propose the new square array without central nanoparticle for $\text{SiO}_2/\text{Au}/\text{SiO}_2$ nanoparticles. Calculations show significant enhancement in power absorption and short circuit current of respectively $\sim 136\%$ and $\sim 154\%$, compared to the structure without nanoparticles. These improvements are justified pursuant to enhanced light trapping inside the active layer.

1. Introduction

Organic photovoltaic devices, in particular, Polymer Solar Cells (PSCs), have attracted more attention due to their unique features such as low manufacturing cost, mechanical flexibility, lightweight and possibility of vacuum-free manufacturing process. These useful features provide opportunities for many new applications (Blom et al., 2007; Changhee et al., 2010; Kippelen and Brédas, 2009; Lipomi et al., 2011; Miyazaki et al., 2005; Park et al., 2011; Zhu et al., 2011). However, Despite the efforts of Ye et al. and the significant improvement in the efficiency of polymer solar cells, PSCs still have lower efficiency compared to perovskite and inorganic solar cells (Minbashi et al., 2017; Omrani et al., 2017; Yang et al., 2017; Ye et al., 2018, 2017a,b). Short electron-hole diffusion length, which is one of the biggest challenges of PSCs, limits the thickness of the absorbent layer (< 150 nm) (Ng et al., 2014). This, in turn, causes the light absorption and short-circuit current (Jsc) to be reduced (Brabec et al., 2001; Dennler et al., 2009). Many research efforts for trapping light inside the cell structure to enhance light absorption have been done. Na et al. increased light absorption and short-circuit current by creating Surface Relief Gratings in

the active layer (Na et al., 2008). Tvingstedt et al. presented a new light trapping structure based on the array of microlenses, which resulted in improving Light absorption and photocurrent by up to 25% (Tvingstedt et al., 2008). Mukul Agrawal in cooperation with Peter Peumans and Richard R. Lunt in cooperation with Vladimir Bulovic, respectively, in 2008 and 2011 were able to enhance light absorption in the active layer using dielectric mirrors (Agrawal and Peumans, 2008; Lunt and Bulovic, 2011). Recent studies have shown that the array of metallic nanoparticles (such as gold and silver) with various forms (nanospheres (Chen et al., 2009; Kim et al., 2008), nanocubes (Ng et al., 2014), nanoprisms (Li et al., 2013; Yao et al., 2014) and nanorods (Hsiao et al., 2012; Lee et al., 2009; Zhang et al., 2014)) inside different layers of solar cell (e.g., hole transporting layer (HTL) (Baek et al., 2013; Haidari et al., 2015; Kozanoglu et al., 2013; Lee et al., 2009; Lu et al., 2012) and the active layer (absorber layer) (Li et al., 2012; Mahmoud et al., 2013; Wang et al., 2011; Xu et al., 2013)) can be efficient as light trap.

When light collides with nanoparticles, free electrons on the surface of the nanoparticles are stimulated by electromagnetic fields and carry out collective oscillation. These oscillations are called localized surface plasmon resonance (LSPR) (Bohren and Huffman, 2008). It depends on

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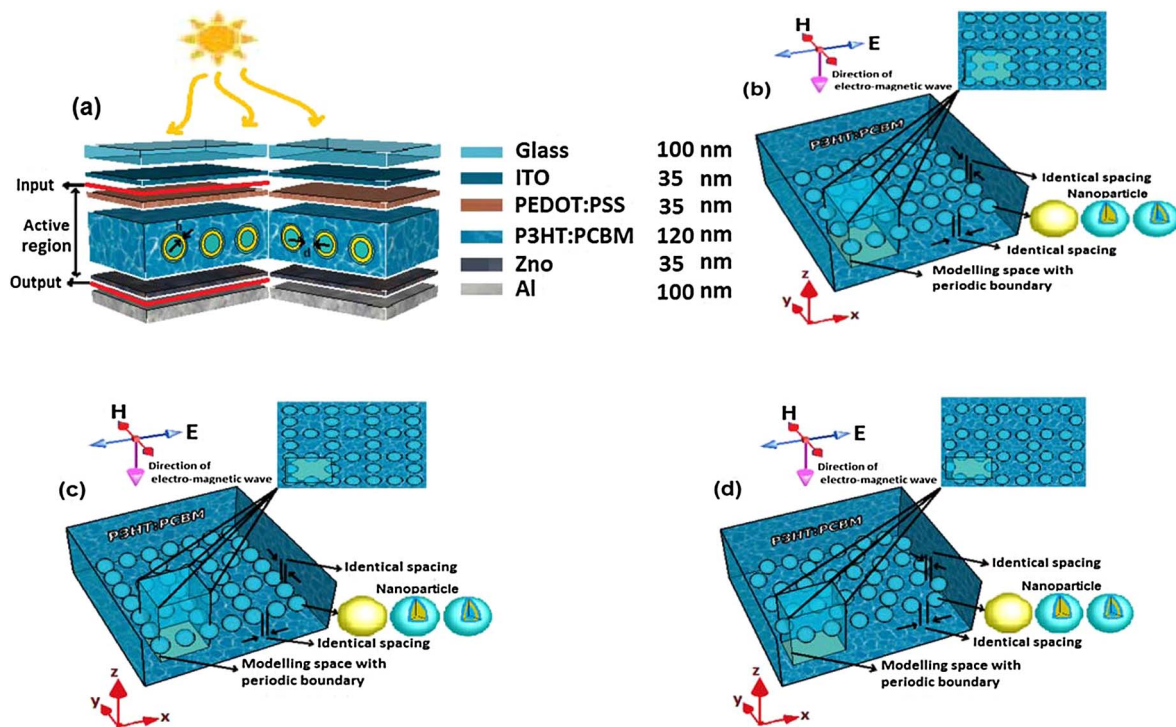


Fig. 1. (a) Model of organic solar cell. (b) Diagram of simulated design of multiple particle with square arrays with central nanoparticle (c) square arrays without central nanoparticle and (d) hexagonal arrays doped in P3HT:PC₆₁BM layer.

the type of material, size and shape of the nanoparticles, and the optical properties of the environment around the nanoparticles, such as the refractive index (García, 2011; Kelly et al., 2003; Sovizi and Omrani, 2017). When the incident light collides with the nanoparticle, its energy is scattered or absorbed by the nanoparticle (García, 2011). Inserting Metallic nanoparticles inside the layers of solar cell causes them to behave as local field enhancers and/or light scatterers, which increases the light absorption without increasing the thickness of the absorber layer by increasing the effective length of the light propagation (Atwater and Polman, 2010; Gan et al., 2013; Stratakis and Kymakis, 2013). However the production of a magnified local field around nanoparticles acts as exciton recombination centers, and as a result, the addition of nanoparticles in the active layer increases exciton recombination. Therefore, these nanoparticles are added inside the hole transporting layer (HTL) (for example poly(3,4-ethylene dioxythiophene): poly(4-styrene sulfonate) (PEDOT: PSS) layer) to prevent direct contact of them with excitons (Jankovic et al., 2013; Kim et al., 2012; Zhang et al., 2016). In this case, inserting nanoparticles in HTL had a poor effect on the efficiency (Ng et al., 2014). Hence, recently some research groups have attempted to insert core-shell nanoparticles, coating a dielectric layer on metallic nanoparticle (metal@dielectric), into active layer or the contact surface between HTL layer and active layer: Chen et al. added spherical Au@SiO₂ core-shell nanoparticles with 50 nm shell thickness inside the (3-hexylthiophene):[6,6]-phenyl-C₆₁-butyric acid methyl ester (P3HT:PC₆₁BM) layer and get a ~16% increased solar cell efficiency (Chen et al., 2013). Xu et al. also synthesized the Au@SiO₂ core-shell nanorods inside the active layer of two structures and increased their efficiency by 12.9% and 26% (Xu et al., 2013). Zhang et al. in 2016 optimized the shell thickness of the Au@SiO₂ core-shell nanorods and selected ~3 nm ultra-thin shell thickness and added an array of them to the interface of PEDOT: PSS and active layer (thieno [3,4-b] thiophene/benzodithiophene (PTB7): PC71BM). They were able to increase power conversion efficiency (PCE) and short circuit current (Jsc) by ~27% and ~28%, respectively (Zhang et al., 2016).

Although the addition of a SiO₂ shell prevents direct contact of

excitons to metallic nanoparticles and consequently reduces the recombination of excitons at the metallic nanoparticle surface, but on the other hand, the presence of the SiO₂ shell limits the light scattering from the surface of the nanoparticles. This, in turn, prevents getting more benefit from LSPR effect in increasing light absorption. In studies that have been done up to now, less attention has been given to this issue. In this work, at first, the effect of adding the SiO₂ shell to spherical metallic nanoparticles on the local field and the light scattering in the P3HT:PC₆₁BM polymeric layer, as well as the effect of inserting a square array of these nanoparticles inside the active layer on power absorption are investigated and the shell's thickness is optimized according to reference (Zhang et al., 2016). Subsequently, by providing a new triple-core-shell structure for spherical nanoparticles in the form of SiO₂@Au@SiO₂, the power absorption and short-circuit current (Jsc) have been improved by increasing the local field and light scattering cross-section. Finally, with studying different arrays of nanoparticle placement, we have tried to enhance trapping of scattered lights and increase light absorption. We were able to increase power absorption and short circuit current by ~136% and ~154%, respectively.

2. Simulation process

2.1. Geometry, materials and boundary conditions

In this study, A model of P3HT:PC₆₁BM solar cell made by spin-coating is studied. This solar cell has 6 layers, which respectively includes a glass cover, transparent conducting film (anode), p-type hole transport layer (HTL), active layer, n-type electron transport layer (ETL) and a cathode (Gao et al., 2015). The optical properties (refractive index, n and extinction coefficient, k) of materials are selected from the data in previous publications (Chen et al., 2015; Ko et al., 2009; Monestier et al., 2007; Palik, 1998; Tumbleston et al., 2008). The glass layer is a substrate, and the other five layers deposited on that layer and are created the solar cell structure. The spherical nanoparticle arrays are placed in the center of the active layer, as shown in Fig. 1. These nanoparticles can be synthesized by using methods referenced in

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