



# Optimization of Nanoparticle Organic Photovoltaic Device Performance using SCAPS Software

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## Abstract

The fabrication of nanoparticle (NP) organic photovoltaic (OPV) solar cells has attracted great interest due to the possibility of controlling the morphology of the active layer and eliminating harmful solvents. However, NP OPV devices exhibit low efficiency compared with bulk heterojunction devices. The solar cell capacitance simulator (SCAPS) simulation package using a framework based on a one-dimensional drift–diffusion model is applied in the current work to improve the efficiency of NP OPV devices with a poly(3-hexylthiophene) (P3HT):phenyl C<sub>61</sub> butyric acid methyl ester (PCBM) active layer. The optimization results confirm that the best thickness for the active layer is 100 nm to 120 nm and that the device reaches its highest performance in this thickness range but low efficiency for thicknesses above 120 nm. Changing the electron mobility (in the range of  $1 \times 10^{-3} \text{ cm}^2/\text{V-s} < \mu_e < 1 \times 10^{-4} \text{ cm}^2/\text{V-s}$ ) is found to have no impact on the device efficiency, whereas the device performance is improved by 27% when the hole mobility is varied in this range ( $1 \times 10^{-3} \text{ cm}^2/\text{V-s} < \mu_h < 1 \times 10^{-4} \text{ cm}^2/\text{V-s}$ ). Additionally, the donor and acceptor density ( $N_D$  and  $N_A$ ) are optimized, revealing that the best values of  $1 \times 10^{15} \text{ cm}^{-3}$  and  $1 \times 10^{18} \text{ cm}^{-3}$ , respectively, lead to an improvement in the device efficiency by about 60%. The current findings indicate that the performance of NP OPV devices can indeed be enhanced by optimizing the morphology of the active layer.

**Keywords** Nanoparticle · organic photovoltaics · SCAPS · effective medium model

## Introduction

Although organic solar cells (OSCs) exhibit low performance and suffer from problems regarding stability, organic materials have become the core of many solar cell devices that have been widely studied by the research community due to their low cost and flexibility, and the possibility of fabricating devices with acceptable power conversion efficiencies of up to 10%.<sup>1,2</sup> Organic materials also present several advantages in comparison with inorganic materials, such as low density and desirable mechanical properties.<sup>3,4</sup> In addition, organic materials can be processed or coated onto various substrates such as glass and flexible substrates by the simple spin-coating method or inkjet printing for small devices, or roll-to-roll fabrication processes for large-scale devices.<sup>5,6</sup> In the organic electronics research community,

great effort has been made to optimize and control the morphology of the active layer, leading to improvements in the overall performance of OSC devices.<sup>7,8</sup> The active layer of OSC devices can be synthesized in three morphologies: bilayer, bulk heterojunction (BHJ), and nanoparticle (NP).<sup>9–11</sup> Based on previous reports, BHJ OPV devices can exhibit efficiencies of 5% to 10%, a key parameter for the commercialization of such organic photovoltaic devices produced by roll-to-roll methods.<sup>12</sup>

Nanoparticle (NP) organic photovoltaics (OPVs) benefit from a water-processable concept for the active layer material, thereby eliminating harmful solvents, as well as the ability to control the semiconducting polymer in addition to preparing nanoscale morphologies.<sup>13</sup> NP-OPVs can thus contribute to addressing environmental, health, and safety issues related to the fabrication process, in contrast to conventional (BHJ) devices.<sup>14,15</sup> The morphology of such materials is typically a core–shell NP structure. A common active layer system for NP-OPV is the poly(3-hexylthiophene) (P3HT):phenyl C<sub>61</sub> butyric acid methyl ester (PCBM) blend, which includes P3HT (~ 70% in the shell)

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