

Review

Performance of poly(3-hexylthiophene) in bulk heterojunction solar cells: Influence of polymer size and size distribution



Jose Jonathan Rubio Arias, Maria de Fatima Vieira Marques *

Universidade Federal do Rio de Janeiro, Instituto de Macromoléculas Eloisa Mano, IMA-UFRJ, Cidade Universitária, Av. Horácio Macedo, 2.030, Centro de Tecnologia, Bloco J., Rio de Janeiro-RJ, Brazil

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ABSTRACT

Poly(3-hexylthiophene) (P3HT) is a versatile polymer that has been deeply studied as a material for electronic devices and also for organic solar cells. This study is a recompilation of the molar mass and polydispersity dependence studies on its charge carrier mobility, crystallinity and PCBM based solar cells. Through the examination of different works, it has been demonstrated the necessity of increasing annealing temperature along molar mass in order to obtain better values of power conversion efficiency. Due to the probable polymer degradation, thermal analysis must be performed in order to approach the observed trend of increasing charge carrier mobility along with molar mass. The maximum power conversion efficiency (PCE) value reported for P3HT: PCBM device is 4.42% for a P3HT with number average molar mass M_n of 43 kDa and polydispersity index (PDI) of 2.1. This latter parameter was found to play an important role in the solar cell performance, and it was observed that a narrow molar mass distribution is not always desirable, especially for polymers with high molar masses.

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Contents

1. Introduction	58
2. Influence of molar mass on performance of polythiophenes	59
3. Influence of molar mass distribution	62
4. Effect of side chain in polythiophenes	63
5. Nanoparticles of fullerene	65
6. Outlook and conclusions	67
References	68

1. Introduction

The contemporary increase in energy demand around the world is gradually becoming a problem for nations, which need to supply enough energy for all its socioeconomic activities [1]. In order to overcome this challenge, new energy sources are in process to be studied nowadays, from nuclear fusion [2,3] to renewable energies like geothermal, wind, maremotriz and solar [4,5]. Solar energy is the one that is growing fastest among the renewable energies [4] (including photovoltaic and solar thermal energy), and this is mainly due to the fact that energy source is free and virtually infinite (in human time scale). Indeed,

the amount of energy that reaches the earth surface in one single hour is 6.23×10^{20} kJ [6], which according with several studies should be enough for satisfying the entire demand of energy for the human civilization in one year [4,7]. This huge amount of energy that strikes the earth surface is one of the main motivations to better explore the solar energy, specially the photovoltaic energy, due to the fact that solar thermal power plants require a dedicated infrastructure [8] while solar panels can be installed anywhere and generate locally the required energy without need of transportation infrastructure [4,9].

One of the main issues of regular solar panels is the high production cost which is related to the purification of silicon, gallium, arsenic, etc., and the vacuum deposition involved in the manufacturing processes [10,11]. Besides that, and in spite of the relatively high values of power conversion efficiency (PCE), the own nature of regular solar panels (high weight, and rigidity) limits its spread for application in

* Corresponding author.

E-mail addresses: jonathanrubio@ima.ufrj.br (J.J. Rubio Arias), fmarques@ima.ufrj.br (M.F. Vieira Marques).

more architecture elements of buildings and vehicles [1]. In order to overcome these issues, new solar cell technologies have been developed. In this context, bulk heterojunction solar cells (BHJSCs) are devices, which are called to make part of the revolution in energy generation, due to its versatility, ease of processability and relative low cost. Those solar cells along with dye sensitized solar cells are meant to be part of new generation of solar cells that can be incorporated to almost every architecture element, including windows, roofs, walls and even coatings for vehicles [9].

BHJSCs are devices that convert the energy contained in photons of sunlight directly into electricity, using an active layer that is capable of absorbing a photon, generating a pseudo particle called exciton, which can undergo two different processes: recombination or charge transfer (Fig. 1). Depending on the morphology of active layer, it will be favored one or either the other process. For a better energy conversion, morphology of BHJ must be appropriate to maximize the charge transfer and minimize the exciton recombination [12,13].

Electron donor structure is fundamental for good performance of BHJ devices and there are several features that depend on that parameter. For instance, polymer solubility (which influences the way in which polymer and electron acceptor interact when solvent is leaving the system); the conjugation length, a parameter extremely important for bandgap; HOMO and LUMO values; and molar mass, which can influence on both conjugation length and solubility as well as crystallinity and charge transportation [14–16].

P3HT is a conjugated electron donor polymer of spread use in BHJ solar cells, due to its good electro-optical properties ease of process and synthesis [17–21]. Its structure, presented in Fig. 2, consists in a main backbone that bonds 3-hexylthiophene molecules at the positions 2 and 5. Along this review, it will be analyzed regioregular polymer, due to the fact that it has been demonstrated that regioregularity has an

intense influence on polymer properties and regioregular polymers show the best performance [22–25].

Molar mass effect on common polymer properties has been studied mainly for purposes of determining its influence on mechanical, chemical and thermal properties; however, it can have a big impact in conjugation length and solubility for conjugated polymers [24–26]. This review aims to collect and correlate all the relevant information reported about P3HT molar mass influence on BHJSCs performance. This study will present the degree of polymerization (DP) in order to aid visualizing the influence of conjugation length, instead of only consider M_n . This is due to the fact that the DP is a key aspect in determining the relationships between number of mers and polymer performance, which helps when it comes to comparison among different polymer structures.

2. Influence of molar mass on performance of polythiophenes

In 1998, Trznadel and co-workers tried the synthesis of P3HT through the Grignard coupling and found through NMR studies that there is some residual isomer of monomer 2-bromo-3-hexylthiophene, namely 2-bromo-4-hexylthiophene that acts as a termination agent, which lowers the final molar mass [27]. Working with DP between 14 and 106, the authors obtained through solvent fractionation mechanism, different polymer molar masses as follow: with acetone (DP = 14), hexane (DP = 26), dichloromethane (DP = 50), and THF (DP = 106), the authors found that the highest conjugation length (corresponding to the highest molar mass) the lowest oxidation potential obtained, which is somehow related to the value of HOMO energy level and thus, increasing the energy bandgap with a consequent reduction on photon harvesting [27].

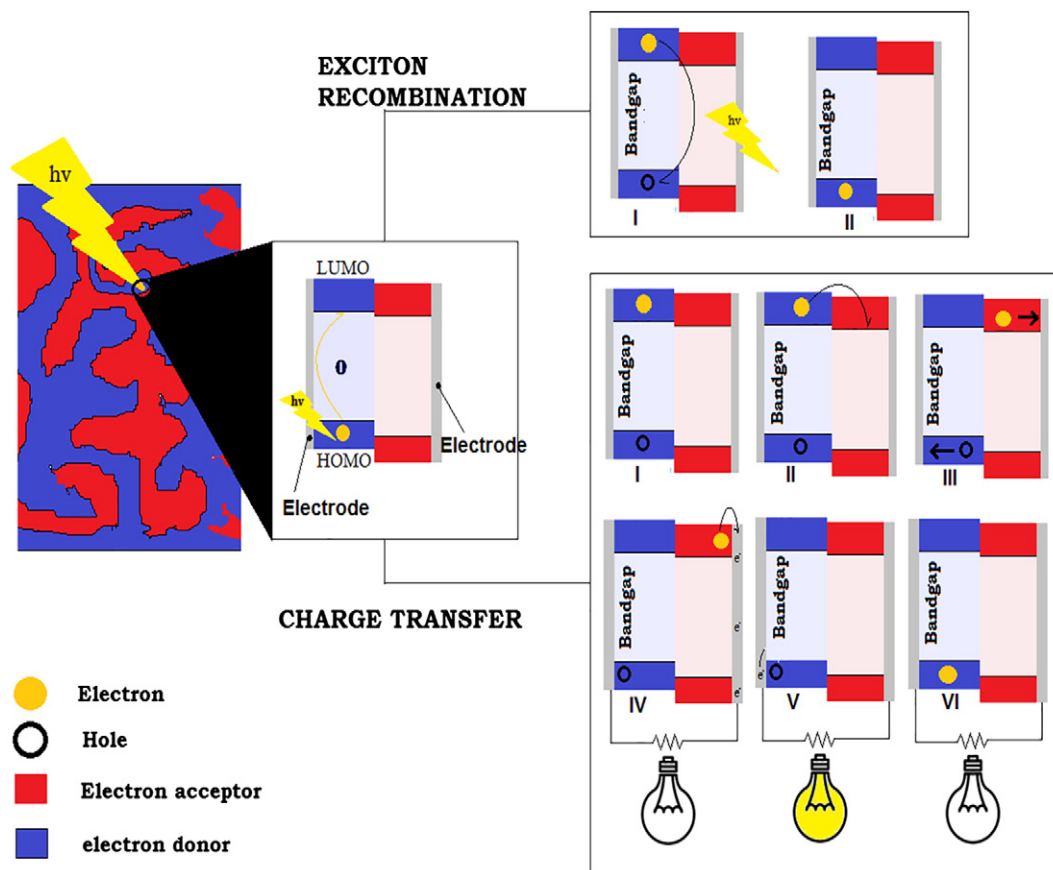


Fig. 1. General schematic representation of recombination and charge transfer processes. The figure represents the incidence of a sunlight photon in a bulk heterojunction and the two possible phenomena that can occur after the photon strike. The numeration from I to VI represents several stages of the charge transfer process.

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