



ELSEVIER

Available online at [www.sciencedirect.com](http://www.sciencedirect.com)

SCIENCE @ DIRECT®

Solar Energy Materials  
& Solar Cells

Solar Energy Materials & Solar Cells 87 (2005) 33–47

[www.elsevier.com/locate/solmat](http://www.elsevier.com/locate/solmat)

# Molecular films based on polythiophene and fullerol: theoretical and experimental studies

M.E. Rincón<sup>a,\*</sup>, R.A. Guirado-López<sup>b</sup>,  
J.G. Rodríguez-Zavala<sup>b</sup>, M.C. Arenas-Arrocena<sup>a</sup>

<sup>a</sup>*Centro de Investigación en Energía, Universidad Nac. Autónoma de México, UNAM,  
Apartado Postal 34, Temixco 62580, Morelos, México*

<sup>b</sup>*Instituto de Física, UASLP, Alvaro Obregón 64, San Luis Potosí 78000, SLP, México*

Received 15 May 2004; received in revised form 29 June 2004; accepted 3 July 2004

Available online 23 November 2004

## Abstract

We report the electrical and optical properties of molecular films made of homogeneous and segregated mixtures of polythiophene with both  $C_{60}$  and  $C_{60}(OH)_{24-28}$  compounds, and relate the trends observed with theoretical predictions based on systematic studies of the electronic structure and energetics of polyhydroxylated fullerenes. The electric and optical properties are strongly correlated to the degree of phase segregation in the molecular films and also to the tendency of the hydroxyl groups to cluster on the  $C_{60}$  cage, thus providing useful information on the potential of hydroxylated fullerenes for the development of buffer layers for fullerene/conductive polymer solar cells. Finally, we underline the importance of quantifying the changes in the electronic structure of the  $C_{60}$  molecules when the chemical functionalization of their surfaces is performed in order to better understand and improve the efficiency of fullerene-based solar cell materials.

© 2004 Elsevier B.V. All rights reserved.

*Keywords:* Solar cells; Molecular films; Fullerol; Fullerene; Polythiophene; PEDOT–PSS

\*Corresponding author. Tel.: +52 555 6229 748; fax: +52 777 3250 018.

E-mail address: [merg@cie.unam.mx](mailto:merg@cie.unam.mx) (M.E. Rincón).

## 1. Introduction

Photovoltaic cells based on thin polymer films have great potential as a cost-effective, renewable, alternative energy source [1,2]. In particular, polymer–fullerene composites are one of the most effective and therefore extensively studied concepts in device design [3,4]. Here, photon absorption takes place in the polymer and forms bound e–h pairs that separate due to the electron-donating nature of conjugated polymers and the electron-accepting nature of C<sub>60</sub>. As it is well known, the precise microstructural features of the films are of crucial importance for the optimal device performance, where photo generation of carriers must be accompanied by its efficient transport and collection [1]. Although blend structures have the maximum interface between donor and acceptor molecules, paths for charge percolation to the electrodes and ohmic contacts at the film/electrode interfaces become limiting factors to device performance. The bilayer structure, on the other hand, has limited interfacial area, however charge transport through the appropriate phase and charge collection at the right electrode are intuitively less complicated.

In the last years, various strategies have been followed to optimize blend structures and handle the weak compatibility of conjugated polymers and C<sub>60</sub>, which causes phase-segregation at high C<sub>60</sub> concentrations [5]. These include chemical functionalization of C<sub>60</sub>, modification of the conjugated polymer, and addition of a third component to acts as a plasticizer. In this paper, we explore the optical, transport, and electronic properties of molecular films made of water-soluble C<sub>60</sub>(OH)<sub>24–28</sub> (fullerol) to establish its potential as buffer layers in typical polymer–fullerene solar cells. In typical devices, poly(3,4-ethylenedioxythiophene)–poly(styrenesulfonate) (PEDOT–PSS) is broadly used to form ohmic contacts with several metals and indium tin oxide (ITO) coated glass substrates. Since it is a water-soluble polythiophene derivative, its polar groups could cause the segregation of the hydrophobic molecules of fullerene derivatives present in the active bulk layer of the device. An amphiphilic molecular layer, with the proper electrical and optical properties, seems adequate to solve this problem. In particular, highly OH-covered fullerene might be a good candidate to consider. They have been already widely synthesized and it has been possible to estimate the number of adsorbed OHs, although it is very difficult to identify the disposition of the hydroxyl groups on the carbon surface. In this respect, previous theoretical studies addressing the electronic and structural properties of polyhydroxylated carbon fullerenes at low coverage [C<sub>60</sub>(OH)<sub>n</sub>, 1 ≤ n ≤ 14] [6], along with experimental evidence of amphiphilic fullerol structures [7], lead to the conclusion that the local organization of hydroxyl groups depends on the number of OHs attached, and that the existence of molecular hydroxyl islands on the surface of C<sub>60</sub> is usually more favorable than a random distribution of OH groups. The theoretical studies also indicated the appearance of new electronic states in the valence region of the spectra having strong oxygen 2p character and causing the decrease of the HOMO–LUMO energy gap respective to the uncovered cage. Therefore, it is possible that amphiphilic molecular films of C<sub>60</sub>(OH)<sub>24–28</sub> could decrease the segregation of hydrophobic fullerene derivatives at the PEDOT–PSS interface, while still keeping its ohmic nature for hole-collection.

Download English Version:

<https://daneshyari.com/en/article/9618652>

Download Persian Version:

<https://daneshyari.com/article/9618652>

[Daneshyari.com](https://daneshyari.com)