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Extended Abstract

Assessment of optical properties of graphene - poly(3-hexylthiophene) nanocomposite applied to organic solar cells †

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Abstract: Poly(3-hexylthiophene) (P3HT) is a p-type organic semiconductor and is intrinsically a donor material. It is one of the most attractive polymers because of its high electrical conductivity and solubility in various solvents. However, its carrier mobility is considered low when compared to that of inorganic semiconductors. In this work, it will be shown how the addition of different graphene (G) contents tailors the principal optical parameters of P3HT such as the bandgap, the hole collection properties, the carrier mobility, the refractive index, and the extinction coefficient. In particular, the hole collection properties and the carrier mobility are enhanced, and the bandgap reduced with increasing graphene content.

Keywords: nanocomposite, refractive index, extinction coefficient, graphene

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1. Introduction

New photovoltaic energy technologies can contribute to environmentally friendly, renewable energy production, and the reduction of the carbon dioxide emission associated with fossil fuels and biomass. A new photovoltaic technology, organic solar cells , is based on conjugated polymers and molecules. Organic solar cells have attracted considerable attention in the past few years owing to their potential of providing environmentally safe, flexible, lightweight, and inexpensive devices [1]. In this context, the efforts are mostly concentrated on increasing power conversion efficiencies and reducing the cost of materials and processing conditions.

Poly(3-hexylthiophene) (P3HT) is a p-type semiconductor and is intrinsically a donor material. P3HT is a regioregular polymer, which means that each repeating unit is derived from the same isomer of the monomer and is one of the most attractive polymers because of its high electrical conductivity and solubility in various solvents. Moreover, P3HT has a high absorption coefficient (on the order of 105 cm^{-1}) and can absorb more than 95% of the solar spectrum over a wavelength range of 450–600 nm when deposited in a 240 nm thick film. This makes it very attractive for organic optoelectronic devices [2]. Moreover, P3HT possesses several other advantages such as solution processability, easy and low-cost fabrication. It also possesses one of the highest electrical mobilities of the known conjugated polymers, 0.2 cm^2 /(V·s). However, this mobility is considered low when compared to those of inorganic semiconductors [3,4].

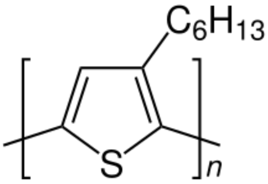

Figure 1. Scheme of P3HT monomeric unit. [4]

Novel acceptor materials, such as graphene (G), a one-atom-thick sheet of sp^2 hybridized carbon atoms arranged in a hexagonal lattice, which was first discovered in 2004 by Novoselov et al. [5] have been intensively investigated given their outstanding electrical, optical, chemical, and mechanical properties. Graphene has an extraordinary electrical mobility of 15000 cm^2 /(V·s), a high specific surface area (ca. 2600 m^2/g), very high electrical conductivity (up to 6000 S/cm) and a transparency of more than 70% over the spectral range of 1000–3000 nm [3]. A single sheet of graphene has superior mechanical properties because of the strong p-bond in its honeycomb crystal lattice structure, with a tensile strength of 130 GPa and a Young's modulus close to 1 TPa [3, 6].

However, the very low responsivity due to its weak light absorption and fast recombination rate has limited the sensitivity of graphene light-sensing devices [3]. Significant efforts have been applied to increase its absorption, among which a feasible way is the combination with light-absorbing materials [6].

Several methods for the preparation of P3HT/G nanocomposites have been reported, including solution mixing and in situ polymerization [7, 8]. The in situ polymerization consists in mixing nanofillers with a liquid monomer or a precursor of low molecular weight. When a homogenous mixture is attained, polymerization is initiated by addition of an appropriate initiator, which is exposed to a source of heat, radiation, etc. [9]. Polymerization is carried out by adjusting the temperature and time. It is a very effective method that allows carbon-based nanofillers to be dispersed uniformly in the matrix, thereby providing a strong interaction between them [8]. However, certain conditions must be fulfilled, including the use of low viscosity monomers, a short period of polymerization, and no formation of side products during the process.

In this work, P3HT/G nanocomposites with different G loadings have been studied. The aim is to assess how the P3HT principal optical properties change in the presence of different G contents. In this sense, the optical bandgap, the hole collection properties and the carrier mobility have been studied. In addition, the refractive index (n) and the extinction coefficient (k) of the different P3HT/G composites have been shown, discussing the influence of G content on these parameters.

2. Results

In this section, the changes in the optical bandgap, the hole collection properties and the carrier mobility as a function of G content is described. Then, the refractive index (n) and extinction coefficient (k) of six nanocomposites with different contents of G is graphed.

2.1. Method

The main optical and electronic properties of P3HT have been studied before and after the addition of graphene. To do this, firstly, an exhaustive bibliographic search has been carried out. Special attention has been paid to those results related to the application of the studied compounds to organic solar cells.

2.2. Optical parameters

2.2.1. Bandgap, hole collection properties and carrier mobility

The bandgap of P3HT is around 1.9 eV, limiting the absorption to wavelengths under 650 nm. In this spectral range, and under AM 1.5G spectrum, only 22.4% of the photons are found. Consequently, decreasing the bandgap leads to an increase in the total amount of photons that can be harvested. However, narrowing the polymeric bandgap results in a reduction in the power conversion efficiency of the cell due to a decrease in the open circuit voltage (V_{oc}). Therefore, a trade-off should be achieved to obtain the optimum bandgap [10].

According to Bkakri et al. [11] and Chang et al. [2], the spectroscopic ellipsometry (SE) analysis proves that the insertion of low graphene content in the P3HT matrix reduces the thickness of the film and the optical bandgap of the P3HT/G nanocomposites. As a result, the optical absorption properties of the solar cell increase in the visible range.

According to Saini et al. [3], nonetheless, there is not a clear trend in the P3HT bandgap variation with the graphene content. There seems to be a slight increase in the bandgap for low graphene content. However, for high graphene loading levels, both the absolute value of HOMO level and the absolute value of LUMO level slightly increase so that the bandgap remains the same. It is convenient to clear out this discrepancy between authors about the bandgap.

According to AbdulAlmosin et al. [12] the use of P3HT/G improves the solar cell efficiency due to the enhanced hole collection in P3HT in the presence of graphene. P3HT/G bulk heterojunction prepared by solution processing possesses the advantages of the high carrier mobility of G and the high visible light absorption of P3HT. Che et al. [13] fabricated a phototransistor consisting of solution processed P3HT/G bulk heterojunction channel. The device exhibited a hole mobility as high as 3.8 cm^2 /(V·s) due to the enhanced charge transport properties of G.

2.2.2. Refractive index and extinction coefficient

In the following section, the evolution of the complex refractive index of P3HT/G with the G content is discussed. The data of Saini et al. [3] for n and k for six nanocomposites with different loads of graphene have been registered.

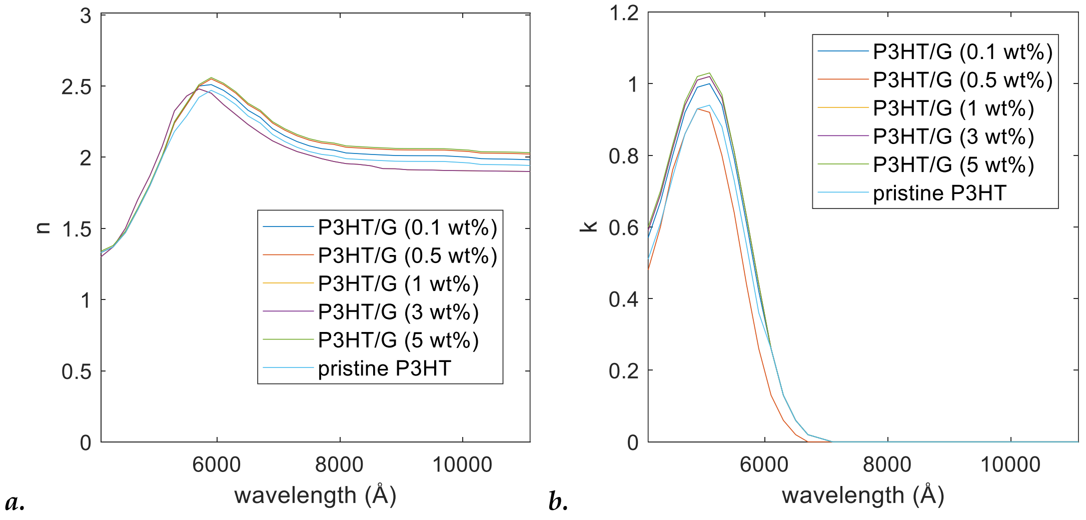

Figure 2. Refractive index (a) and extinction coefficient (b) obtained from ellipsometer analysis for P3HT/G nanocomposites with different G loads [3]

Figure 2a shows the refractive index of these six nanocomposites. It can be seen how n of P3HT with higher loads of graphene is higher, excepting the nanocomposite P3HT/G (0.5 wt%), which n is lower. Regarding k, as is shown in figure 2b, the extinction coefficient of G/P3HT increases with the load of graphene, excepting the case of P3HT/G (0.5 wt%), in which k is lower.

3. Conclusions

In this work, the influence of graphene content in G-P3HT on the optical and electrical properties of the compound has been assessed.

The addition of different graphene (G) contents to P3HT, tailors its main optical parameters. In particular, the hole collection properties and the carrier mobility are enhanced, and the bandgap reduced with increasing graphene content.

It has been found that the refractive index of P3HT generally increases with increasing graphene loading; analogous trend has been found for the extinction coefficient of P3HT/G nanocomposites, with increases steadily with increasing graphene loading.

This preliminary study shows the great potential application of these nanocomposites in organic solar cells. Future work will be carried out to further assess in more detail their optoelectronic properties.

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