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Electroluminescence yield from exciton dissociation in organic-inorganic layers

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Abstract

In this work, we report the electroluminescence yield from exciton dissociation in organic-inorganic layers. The theoretical approach for electroluminescence has been based on the exciton dynamics of the Frenkel exciton and Wannier exciton density. The results indicate that the electroluminescence intensity has been significally reduced by the Förster transfer mechanism. We have found good agreement with experimental results observed in organic MEH-PPV and inorganic CdSe nanoparticles. These findings suggest that this hybrid material could be a promising candidate for optoelectronic devices.

Keywords: Electroluminescence, nanocomposite, Exciton theoretical Approach.

I. Introduction

Recently, organic-inorganic nanocomposites have been presented distinct attention for both experimental and theoretical studies [1-7]. In fact, the incorporation of CdSe nanoparticles (Nps) into polymer MEH-PPV matrix has offered exceptional consideration in organic light emitting diodes (OLEDs) and photovoltaic solar cells [8-11]. This is due to the fact that the incorporation of Nps in polymers can increase brightness and enhance the performance of the OLEDs [12-14]. MEH-PPV is a p-type conjugated polymer (electron donor) it has been considered as one of the first polymers used for polymer-based light-emitting diode applications [15-18]. In the literature, a significant quenching of light emission has been detected with increased CdSe Nps concentration in (MEH–PPV) [19]. It is well known that there is currently no comprehensive theory on exciton dynamics in organic-inorganic nanocomposites. The difficulty in modeling the dynamics of these excitons in nanocomposites is due to three main reasons. The geometry of the nanocomposite is very complicated, because the dispersion of Nps in the polymer matrix is uncontrollable. In the hybrid structures, phenomena at the polymer-nanoparticle interface can give rise to energy and charge carrier transfers, the importance of which can modulate the emitted fluorescence. The excitation of the nanocomposite can generate

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two types of excitons which can emit individually but which can interact with each other and with other elementary excitations in the nanocomposite. In this study, we would like to develop a theoretical model to describe the Nps concentration, the exciton density profiles and the EL intensity in the device. We have chosen the hybrid structure such as (MEH-PPV-CdSe) as an example. Based on the transport and diffusion of the charge carrier in the nanocomposite, the exciton creation, the Förster energy transfer between polymer and nanoparticles and finally the light emission in the hybrid material. In particular, the exciton density profiles in the emissive layer of the nanocomposite are performed for different parameters such as the concentration of injected charge carriers, the Nps capping thickness layer and the Förster transfer rate. Finally, we believe that one of the key design aspects of (Nps-OLED) performance can be associated to the optimal concentration of Nps which lead to high light emission intensity.

II. Photoluminescence and Electroluminescence spectra and Exciton theoretical approach

The electroluminescence process charge injection from an electrode and charge carrier transport are presented in Figure 1. In this work, we have used (CdSe Nps embedded in a MEH-PPV layer) as a hybrid material and (ITO) as anode and (Al) as cathode. The polymer (MEH-PPV) is considered as one of the most popular polymers for hybrid electroluminescent devices [20].

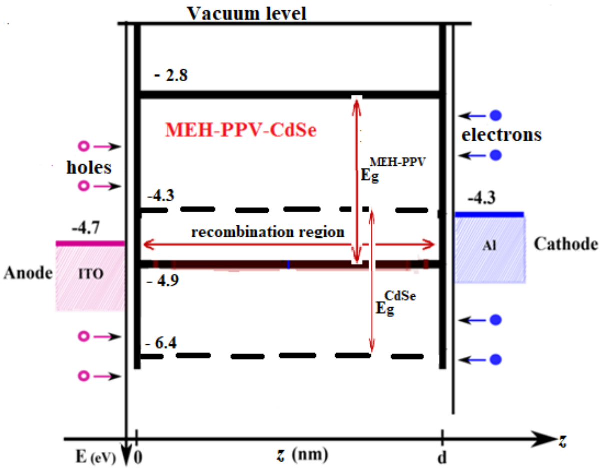

Fig. 1. Schematic view of the hybrid diode ITO/MEH-PPV-CdSe/Al. Eg are respectively the bandgap of the polymer MEH-PPV and the CdSe Nps.

The photoluminescence (PL) and electroluminescence (EL) spectra for different CdSe concentrations (5%, 10% and 20%) are shown in Figure 2. It is noted that the photoluminescence intensity decreases considerably with increasing CdSe concentration and the PL and EL maxima are located around 580 nm and shift slightly towards longer wavelengths as the concentration increases.

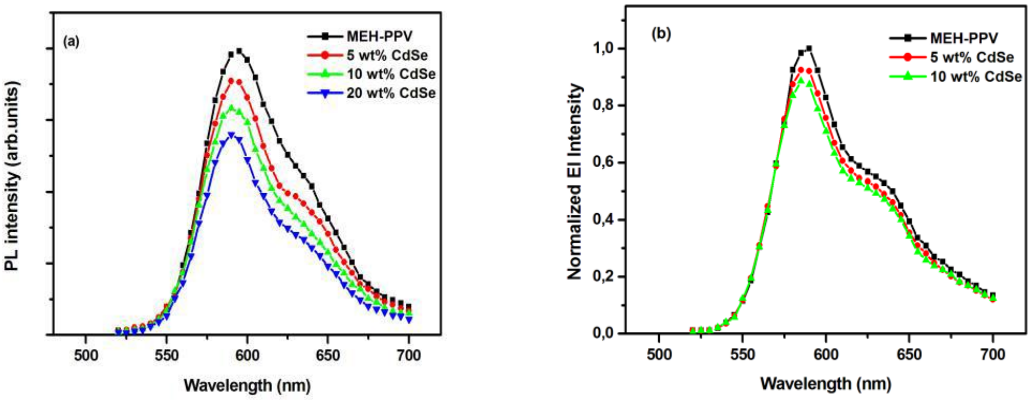

Fig. 2. (a) PL spectra of MEH-PPV-CdSe nanocomposite containing 5%, 10%, and 20% CdSe Nps. *(b) EL spectra of ITO/(MEH-PPV-CdSe)/Al nanocomposites [21].*

In order to control the dispersion and concentration of CdSe Nps in the organic layer, we assume that the carrier mobility is not taken into account:

$$\frac{\partial N_e(z,t)}{\partial t} = D_e \frac{\partial^2 N_e(z,t)}{\partial x^2} - \frac{1}{\tau_e} N_e(z,t) \qquad (1)$$

$$\frac{\partial N_h(z,t)}{\partial t} = D_h \frac{\partial^2 N_h(z,t)}{\partial x^2} - \frac{1}{\tau_h} N_h(z,t) \qquad (2)$$

Where $N_e(z,t)$ and $N_h(z,t)$ are the electron and hole density, $D_{e,h}$ are the electrons/holes diffusion coefficients and $\tau_{e,h}$ describe the electrons/holes effective decay time with the diffusion length for the injected electrons/holes are $L_{e,h} = \sqrt{D_{e,h}\,\tau_{e,h}}$.

In the hybrid materials (CdSe-polymer), the electrons and holes migrate from the cathode and anode through the organic transport layers, where they form excitons.

In order to study the reduction in the light intensity it is necessary to estimate the exciton density profiles in the emissive layer of the nanocomposite for different parameter such as the Förster transfer mechanism, the concentration of injected charge carriers and the capping layer thickness. Therefore, these parameters can also give some information about the material choice for device applications. The exciton density profiles can be deduced from Eq. (1,2) for z spatial coordinate [22]:

$$\frac{\partial N_{exc}(z,t)}{\partial t} = D_{exc} \frac{\partial^2 N_{exc}(z,t)}{\partial z^2} - \frac{N_{exc}(z,t)}{\tau_{exc}} - F_{exc}(z-z_0)\,N_{exc}(z,t) + gI_0 e^{-\alpha z} \qquad (3)$$

where $N_{exc}(z,t)$ represent the exciton density with z the spatial coordinate of exciton propagation between the electrodes, D_{exc} the diffusion coefficient, τ_{exc} the life time of the excited state with exciton diffusion length $L_{exc} = \sqrt{D_{exc}\,\tau_{exc}}$, g is efficiency of light absorption I_0 is the incident photon flux, and α is absorption coefficient. The term $F_{exc}\left(z - z_0\right)N_{exc}\left(z,t\right)$ in Eq. (3) represents the Förster transfer mechanism between the polymer MEH-PPV and Nps. In steady state regime, Eq. (1,2,3) can be written as:

$$N_e(z) = A_e\,e^{z/L_e} + B_e\,e^{-z/L_e} \tag{4}$$

$$N_h(z) = A_h\,e^{z/L_h} + B_h\,e^{-z/L_h} \tag{5}$$

$$N_{exc}(z) = gI_0\left[Ae^{k_{exc}z} + Be^{-k_{exc}z} + e^{-\alpha z}\right] \tag{6}$$

where $k_{exc} = \sqrt{\frac{1}{D_{exc}}\left(F_{exc} + \tau_{exc}^{-1}\right)}$, and the constants A_e, B_e, A_h, B_h, A_{exc}, B_{exc} can be determined *by* the boundary conditions no exciton creation $N_{exc} = 0$ at the bord of the electrodes on $z = 0$ and $z = d$. Figure 3 shows exciton density profiles according to Eq. (6) for different parameter values.

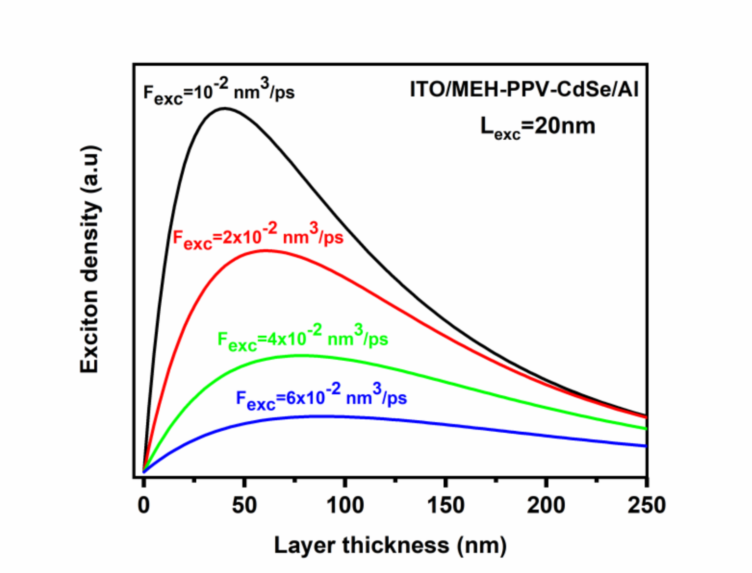

Fig.3. Exciton density profiles versus distance *x* from the ITO and Al electrodes for various Förster transfer rate.

The maximum exciton density has been obtained at a distance $\left(25 \le z \le 50\right)nm$ from the ITO and Al electrodes. This position of the maximum exciton density is dependent on the exciton diffusion length L_{exc}, the Förster transfer rate for the exciton diffusion length is of about $L_{ex}=20$ *nm*. A significant reduction of the exciton density has been shown when the Förster transfer mechanism increases. However, the El quenching can be explained by this mechanism. This is in agreement with reference [18,21] that recommended the quenching attributed to the dominance of Förster energy transfer between host polymer (donor) and guest CdSe nanocrystals (acceptors).

III. Conclusion

In this work, we have performed an analysis of light emission in (polymer-Nps) nanocomposite. By taking into account the density of injected charge carriers, the Förster transfer mechanism, and the excitons density profiles, we found that the reduced intensity in the nanocomposites is caused essentially by the Förster energy transfer between the donor (MEH-PPV) and the acceptor (CdSe Nps) which lead to non-radiative recombination.

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