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Effects of Magnetic Field on the Energetic Behaviors of Excitons in Hybrid Organic-Inorganic Parabolic Quantum Dots

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ABSTRACT

Inorganic-organic hybrid materials have attracted a lot of interest due to their potential application in optoelectronic devices. To understand the basic properties of this new type of nanocomposite, dispersion energies of mixing exciton at the interface in polymer- parabolic quantum dots are theoretically investigated taking into account the interaction between Frenkel and Wannier-Mott exciton. In particular, the effects of magnetic field on the energetic behaviors have been focused to the interaction parameter. Our interest is based to compare the performance of three nanocomposites such as organic P3HT incorporated respectively with inorganic (CdSe, ZnSe, ZnO) parabolic quantum dots. The application of magnetic field induce that the interaction parameter rate increases considerably which can improve the resonance of hybrid exciton. The results indicate that the prominent nanocomposite is essentially related to the P3HT-ZnO.

Keywords: Excitons, nanocomposites, magnetic field, optoelectronic devices, etc.

1. INTRODUCTION

Advances in the research of hybrid organic-inorganic quantum dots semiconductors have given rise to extensive research activities [1-7]. Using the nanocomposites such as CdSe, ZnSe and ZnO inorganic quantum dots embedded in the poly (3-hexylthiophene) (P3HT) more results are important [8,9]. In particular, the interaction of Wannier-Mott-Frenkelexcitons in the hybrid can be described with the coupling term which has been investigated in this work with and without the effect of magnetic fields. Well for these nanocomposites, where the resonant mixing of Wannier-Mott and Frenkelexciton can appear, exciton weights and dispersion energies have been investigate. Moreover, since the Wannier-excitons in quantum dots possess a large Bohr radius, there is why they are sensitive to external perturbations [8, 9]. After having an idea about the energetic behavior of exciton without fields we develop calculation to study the influence of the magnetic field in the electron and hole radius. Some recent control methods are discussed in [18-23].

2. THEORETICAL MODEL

The method of calculation has been used to describe the energetic behaviors of Wannier-Mott-Frenkelexciton formed in the hybrid inorganic–organic device [10, 11]. However, the measurement of the best condition for coupling term is treated with and without magnetic fields. In this work, we consider that the two types of excitonWannier-Mott in quantum dots and Frenkelexcitons in the organic polymer are moving between lattice sites.

The total Hamiltonian of the hybrid system under applied magnetic field B is governed by:

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$$H_{hy} = H_F + H_W(E,B) + H_{Int}(E,B)$$

H_{int} is the interaction Hamiltonian between Wannier-Mott-Frenkelexcitons, which will lead the hybridization by a coupling term constant that defined in (Eq. 1)

$$\Gamma(k,F) = \langle \psi_F | H_{Int}(k,F) | \psi_W \rangle \tag{1}$$

H_{Int} is The Hamiltonien of interaction, $|\psi_F\rangle$ and $|\psi_W\rangle$ describes respectively the Frenkel and Wannier-Mott excitons state.

The most important result of the resonant interaction between Frenkel and Wannier-Mott excitons can be deduced for the large value of the coupling term Γ with wave vector kR_0. Thus the coupling term given in (Eq. 2) as a function of both wave function and electric-magnetic fields is given by the expression:

$$\Gamma(k,F) = \frac{\sqrt{2}\pi\,\mu_W\,\mu_F}{a\varepsilon R_W} k \sqrt{\frac{R_e R_h}{R_e^2 + R_h^2}} \exp\left(\frac{-z_e^2 - z_h^2 + 2z_e z_h + k^2 R_e^2 R_h^2 - 2kR_e^2 z_h - 2kR_h^2 z_e}{2\left(R_e^2 + R_h^2\right)} \right)$$
$$\left(erf\left(\frac{\left(kR_e^2 R_h^2 - R_h^2 z_e - R_e^2 z_h\right)}{R_e R_h \sqrt{2\left(R_e^2 + R_h^2\right)}} + z_0 \frac{\sqrt{R_e^2 + R_h^2}}{\sqrt{2} R_e R_h} \right) - erf\left(\frac{kR_e^2 R_h^2 - R_h^2 z_e - R_e^2 z_h}{R_e R_h \sqrt{2\left(R_e^2 + R_h^2\right)}} \right) \right) \exp\left(-kz_0\right) \tag{2}$$

It's clear that z_e and z_h consider the displaced along (z-axis) of the harmonic oscillators corresponding of the wave functions. R_e and R_h are similar of the effective radius to the electron and hole in the quantum dot which we have to identify their equations next.

The calculations are interested for parabolic quantum dots parameters (CdSe, ZnSe, ZnO) given as a function of the weights according to the Frenkelexciton $\left|C_F(k)\right|^2$ (Eq. 3) and Wannier-Mott exciton $\left|C_W(k)\right|^2$ (Eq. 3) written as:

$$\left|C_F(k)\right|^2 = \frac{\left|\Gamma(k)\right|^2}{\left[E_F(k) - E_{U,L}(k)\right]^2 + \Gamma(k)^2} \tag{3.a}$$

$$\left|C_W(k)\right|^2 = \frac{\left[E_F(k) - E_{U,L}(k)\right]^2}{\left[E_F(k) - E_{U,L}(k)\right]^2 + \Gamma(k)^2} \tag{3.b}$$

Here E_w is the energy of Wannier-Mott exciton and $E_{U,L}$ the energies of the hybrid exciton at the interface of the parabolic quantum dot and the organic crystal [8].

After observed the interaction behaviors corresponding to the coupling term Γ results we are project our work to observe the transformation of the exciton by using the profiles of the hole and electron radius related in (Eq. 4, 5) along the magnetic field given by :

$$R_h(B) = \sqrt{\hbar / m_h \omega_h(B)} \tag{4}$$

$$R_e(B) = \sqrt{\hbar / m_e \omega_e(B)} \tag{5}$$

We note that ω_e and ω_h are the effective frequency upon application of the magnetic field and m_e, m_h are respectively the effective mass of electron and hole.

3. RESULTS AND DISCUSSION

Results are taken for nanocomposites CdSe, ZnSe and ZnO (Qds) embedded in P3HT using the numerical values of parameters depicted in Table.1.

Table1
Physical parameter values of CdSe, ZnSe and ZnO quantum dots use in this work. Typical values for the electric dipole moment of the organic molecular transition *P*, the vector related to the transition of polarization in the solid *D*, the lattice constant of organic crystal *a*, the radius R_0 and the space z_0 are *P=5* Debye, *D=12* Debye, *a=5* Å, R_0=*10*Å, z_0=*20* Å, respectively [8].

Material	ε	R_{Qd} (Å)	m_e^*	m_h^*	R_B (Å)	E_g (eV)
CdSe	9.5	23	0.13	0.74	46	1.74
ZnSe	8.7	17	0.157	0.935	34	2.69
ZnO	8.2	12	0.28	0.54	24	3.2

Following the coupling term Γ G developed in Eq (2), Fig. 1 illustrates the coupling term of P3HT-(CdSe, ZnSe and ZnO) exciton profiles deduced as a function of the wave vectors KR_0. Notice that the coupling term decreasesrespectively for P3HT-ZnO, P3HT-ZnSe and P3HT-CdSe nanocomposites. This is reported previously by the confinement process which is justified by the large Bohr radius in the quantum dots.

The coupling term G has its maximum value in the Brillouin zone with small wave vectors, which is due to the parabolic shape of quantum dot. The exciton behaviors tend to Wannier-Mott exciton state, and they possess the larger radius like the Bohr radius [12-15]. Therefore we have good results of coupling term for nanocomposite P3HT-ZnO which corresponding to the less values of quantum dot core radius and exciton Bohr radius (seeing Table1.).

After having a view for interaction behaviors, Eq(3) and Eq(4) are developed to discuss the best condition to obtain more recombination for Wannier-Mott-Frenkelexciton . Here we can deduce the resonance state

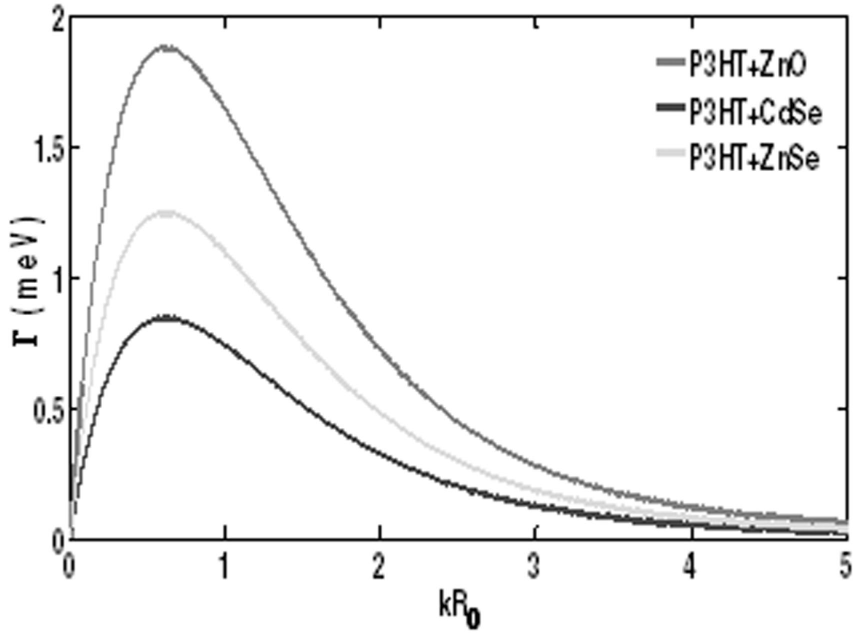

Figure1: Coupling term G for nanocomposite P3HT-(CdSe, ZnSe, ZnO).

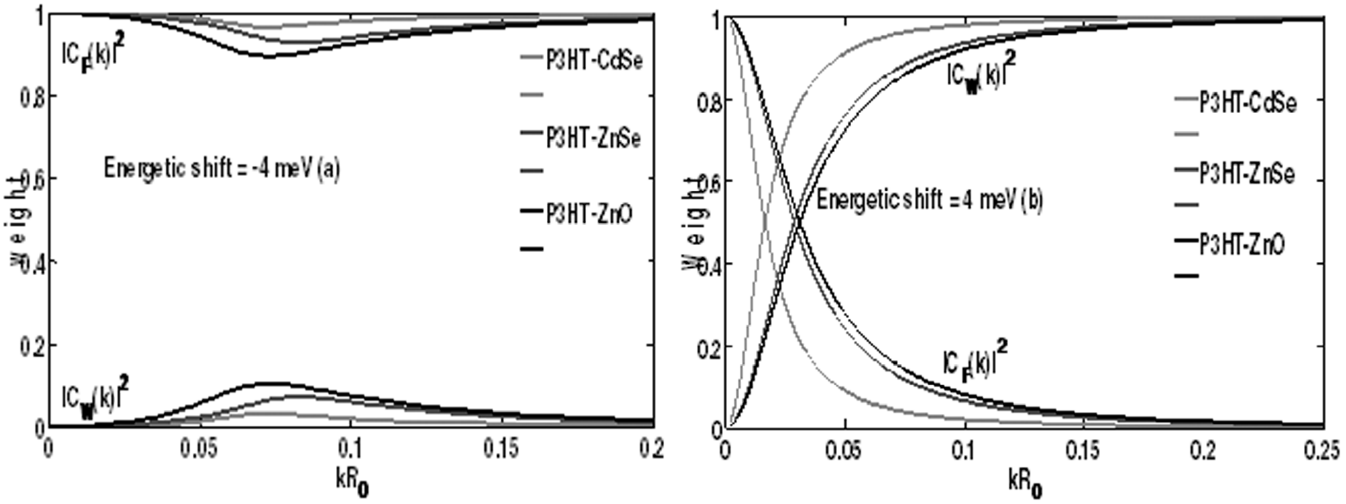

Figure 2: Weights $|C_F (K)|^2$ and $|C_W (K)|^2$ for the lower hybrid Frenkel-Wannier-Mott exciton state for a positive and negative energetic shift (a. $\Delta = -4$ meV, b. $\Delta = 4$ meV).

of the two excitons by express the results with two values of energetic shift " between the Frenkelexciton and the fundamental Wannierexciton level. We show that $\Delta = E_W(0)-E_F(0)$ and the Frenkelexciton is independent of the in-plane wave vector K. In this case the Wannier-Mott $|C_W (K)|^2$ and Frenkel $|C_F (K)|^2$ exciton weights are gives in Fig. 2 (a, b) for $\Delta = \pm 4$ meV;

It is clear that the weights $|C_F (K)|^2$ corresponding to Frenkelexciton taking in Fig. 2. (a, b) near zero wave vector and for energetic shift $\Delta = \pm 4$ meV predominant and decreases for large wave vectors KR_0. On the other side the Wannier-Mott exciton $|C_W (K)|^2$ gives zero and increases in the same area.

In Fig. 2. (b) for $\Delta = 4$ meV we have $|C_W (K)|^2 = |C_F (K)|^2$, well $\Gamma (K) = |E_F(K)-E_W(K)|$ which corresponds at a strong coupling between the Frenkel and Wannier-Mott energies. We note that the hybrid excitonic shifts become clear and corresponding approximately to the resonance [14-19]. Finally, an important effect is the possibility of using energetic shift $\Delta = 4$ meV for tune the resonance between Frenkel and Wannier-Mott excitons, so we have to complete the calculation with this value of energetic shift.

Passing to the Fig. 3(a, b, c), we discuss the results of the coupling term under applied the magnetic fields B. We show that Fig. 3 is corresponding to the nanocomposite P3HT-((a) CdSe, (b) ZnSe and (c) ZnO) as a function of wave vectors kR_0.

Note that, at small radius R_0, the coupling term curves are mainly fixed by the quantum size effect and these results are nearly the coupling term. On the other hand, at large wave vectors kR_0, the exciton states appears and the magnetic confinement affects the size of the coupling term from B = 1T to B = 5T.

Consequently, we should mention that (Fig.3c) corresponding to the nanocomposite P3HT-ZnO has the best results for the application of magnetic fields. This is due to the fact that the exciton recombination has a maximum value in the nanocomposite P3HT-ZnO unlike the charge recombination in the others. To understand the increases of coupling term as function as large values of magnetic fields, we assimilate this result to the fact that we will have best extraction of charges. In this case we can previously deduce that the recombination between electrons and holes is increasing taken so it created more population of excitons.

To demonstrate the influence of magnetic fields in the nanocompositeexciton radius, we have focused our attention to calculate the hole and electron radius using Eq. (7, 8) for CdSe, ZnSe and ZnOQds added to P3HT which is presented in (Fig. 4).

We obtain a remarkable difference between the extension of the electron R_e and hole R_h in the Qds under the magnetic field effect for $R_0 = 80$ Å. Therefore we can understand by the results of calculations

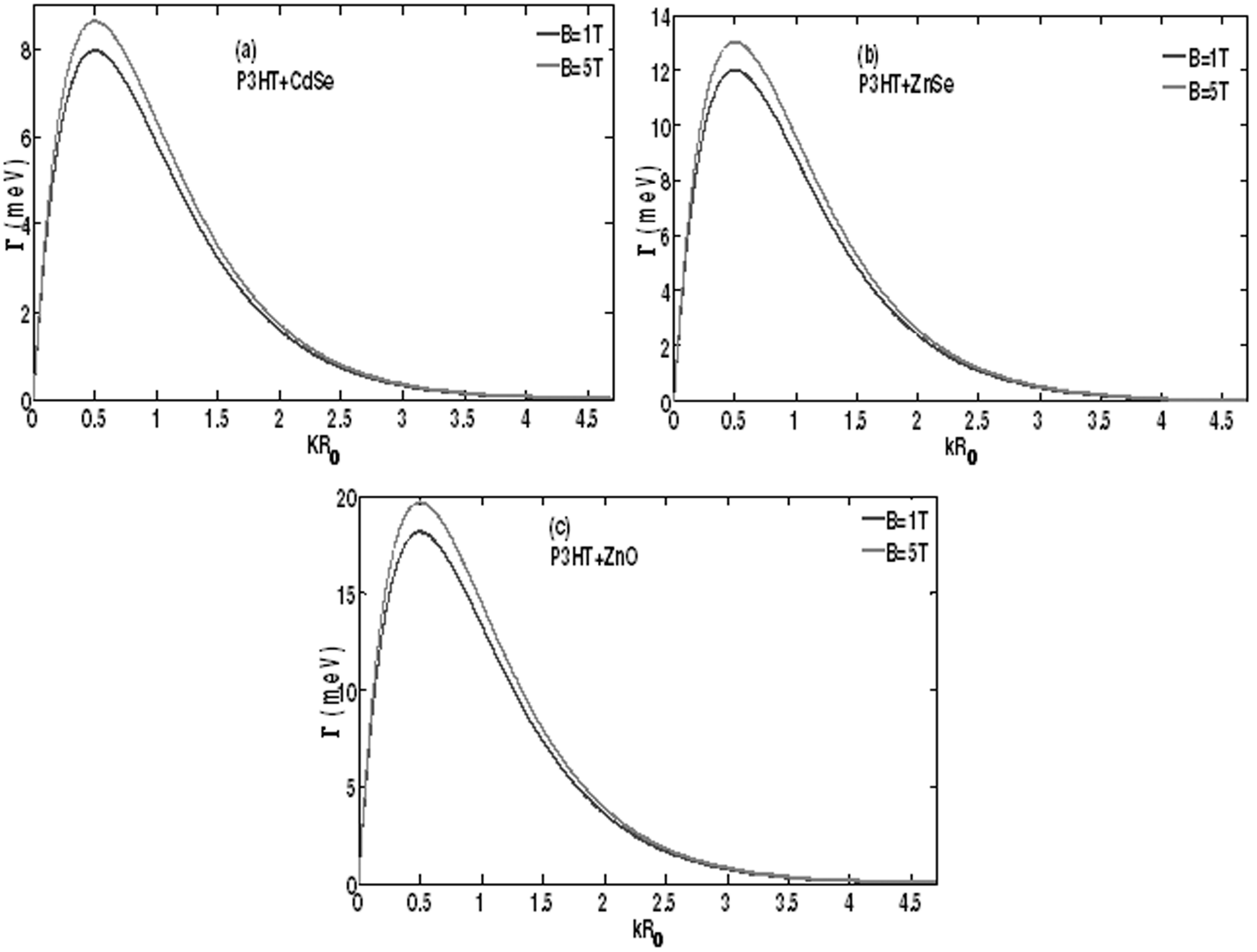

Figure3: Coupling term for nanocomposit P3HT-((a) CdSe, (b) ZnSe, (c) ZnO) as a function of KR_0 for two differents values of magnetic field B for R_0 = 40 Å and z_0 = 55 Å.

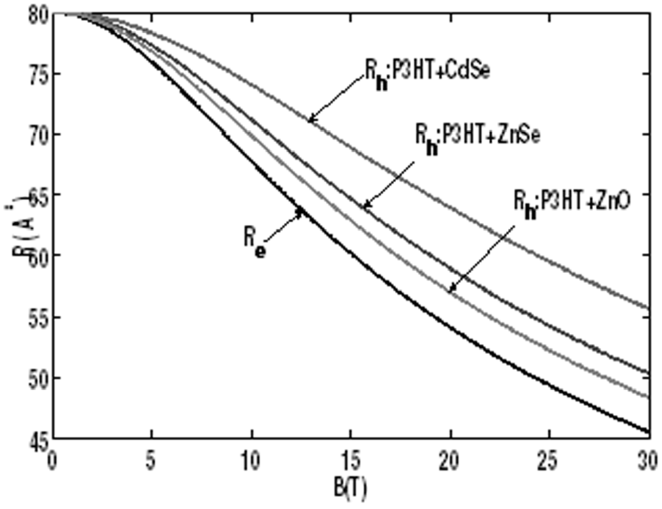

Figure4: Change of effective widths corresponding to the electron R_e and hole R_h quantum dots according to the magnetic field B for R_0= 80 Å.

that more recombination of charges is found in the nanocomposite P3HT-ZnO by comparing to the others electron-hole radius in P3HT-ZnSe and CdSe-P3HT. We notice also that the electron and hole radius decrease with the largest values of magnetic field. It is due to the extra confinement of the magnetic field when it is created and it is observed that the effect of magnetic field will have more influence for the bigger radius than the smaller ones. We should focus that for large magnetic fields we can have the best results of hybrid devices.

4. CONCLUSION

We have demonstrated with the nanocomposite structures of various quantum dots (CdSe, ZnSe and ZnO) mixed in polymer P3HT that the behaviors of coupling terms have interest results under magnetic fields effects. This work confirmed that the coupling term have the same behavior of the leader of confinement corresponding to the Wannier-Mott excitons which is very sensitive to external fields. In this case we have demonstrated that this coupling increases with the magnetic field effects, so the confinement has been affected. Calculations are investigated to describe the weights of excitons as functions as values of energetic shift between the Wannier-Mott-Frenkelexcitons. Lastly we agreement the results of the magnetic field influence to the hole and electron radius to show that magnetic fields reaches the recombination of electrons and holes which ameliorates the coupling term. Further work is in progress to according our theoretical results of the effect of electric and magnetic fields with experimental data and we will observe in the final the benefits of hybrid devices.

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