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Dependence of Exciton Diffusion Length and Diffusion Coefficient on Photophysical Parameters in Bulk Heterojunction Organic Solar Cells

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Abstract

Recently, the dependence of exciton diffusion length (L_D) on some photophysical parameters of organic solids has been experimentally demonstrated, however no systematic theoretical analysis has been carried out in this direction. We have carried out a theoretical study by using the Förster resonance energy transfer and Dexter carrier transfer mechanisms together with the Einstein-Smoluchowski diffusion equation to derive analytical models for the diffusion lengths (L_D) and diffusion coefficients (D) of singlet (S) and triplet (T) excitons in organic solids as functions of spectral overlap integral (J), photoluminescence (PL) quantum yield (ϕ_D), dipole moment (μ_T) and refractive index (n) of the photoactive material. The exciton diffusion lengths and diffusion coefficients in some selected organic solids were calculated, and we found that the singlet exciton diffusion length (L_D^S) increases with ϕ_D and J, and decreases with n. Also, the triplet exciton diffusion length (L_D^T) increases with ϕ_D and decreases with μ_T. These may be achieved through doping the organic solids into broad optical energy gap host materials as observed in previous experiments. The calculated exciton diffusion lengths are compared with experimental values and a reasonably good agreement is found between them. The results presented are expected to provide insight in synthesizing new organic solids for fabricating bulk heterojunction (BHJ) organic solar cells (OSCs) yielding better power conversion efficiency (PCE).

Key words: Exciton diffusion length, diffusion coefficient, Föster resonance energy transfer, Dexter carrier transfer, photophysical parameters, photoactive materials.

Introduction

In the past few decades, organic solar cells (OSCs) have attracted remarkable interest owing to their promising features such as lightweight, large area production, easy fabrication, mechanical flexibility and cost-effective alternatives to commercial-scale electricity generation plants like fossil fuel powered generators, and nuclear power plants [1,2]. Many researchers and engineers believe that the power conversion efficiency (PCE) of OSCs should reach 10-15% before they can be commercialized [1-3]. One of the most efficient OSCs at present is the bulk heterojunction (BHJ) OSC, which consists of a blend of organic donor material and fullerene acceptor as the active layer sandwiched between two electrodes. Although the efficiency of BHJ OSCs has reached more than 10% [2], one still needs to understand the energy loss mechanisms in the operation of OSCs, which are known to reduce their efficiencies [1,2].

In BHJ OSCs, Frenkel excitons can arrive at the interface by diffusion if the exciton diffusion length (L_D) is larger than the distance to the donor and acceptor interface. At the interface an exciton created by a donor molecule can transfer its electron to the acceptor molecule, which has a lowest unoccupied molecular orbital (LUMO) with a lower energy and an exciton excited in the acceptor can transfer its hole to the donor's highest occupied molecular orbital (HOMO) being at a lower energy. Such excitons with electron in the acceptor (A) and hole in the donor (D) are called charge transfer (CT) excitons. These CT excitons need to be dissociated into free electron (e) and hole (h) which can be collected at the opposite electrodes to generate photocurrent. In order to achieve efficient dissociation of excitons excited in the donor, the energy difference between the LUMO of the donor material $(E_{\text{LUMO}}^{\text{D}})$ and LUMO of acceptor material $(E_{\text{LUMO}}^{\text{A}})$, called LUMO energy offset (ΔE_{LUMO}), must be larger than or equal to the exciton binding energy (E_B), that is $\Delta E_{\text{LUMO}} \geq E_B$. Likewise, for efficient dissociation of excitons excited in the acceptor, the HOMO energy offset, $\Delta E_{\text{LUMO}} = E_{\text{HOMO}}^{\text{D}} - E_{\text{HOMO}}^{\text{A}}$ should be greater or equal to E_B. Typically, the exciton diffusion length in organic semiconductors is only a few tens of nanometers [4]. Excitons formed at a distance from the interface longer than the diffusion length will recombine before reaching the interface, resulting in no CT excitons and hence no exciton dissociation. Therefore, the blend of heterojunction should be such that the interface between the donor and acceptor is within the exciton diffusion length.

In BHJ OSCs, it is always advantageous to choose organic materials which have longer L_D, and therefore one needs to know how L_D depends on material parameters. Until now, the most explored approach to optimize L_D is to decrease the donor-acceptor separation distance [5-10]. Several theoretical and simulation works have also been performed over the past few years [11,15-19]. Recently, Stehr et. al. [11] proposed a theoretical model to calculate the singlet exciton diffusion length based on Marcus theory that employs a quantum chemical method. According to this model, the singlet exciton diffusion lengths, $L_D^S=18$ nm in naphthalene and $L_D^S=12$ nm in anthracene are far lower than their corresponding measured values $L_D^S=48$ nm [12] and 60±10 nm [13], respectively, but in diindenoperylene (DIP) the singlet exciton diffusion length was found to be 103 nm, which agrees better with the corresponding experimental value $L_D^S>100$ nm [14]. It could be deduced from their results that the Marcus theory exhibits better performance for exciton diffusion in DIP but underestimates the L_D^S values of naphthalene crystal. Tamura and Matsuo have recently [15] calculated the singlet exciton diffusion length in tetrabenzoporphyrin (BP) by applying Fermi's golden rule and the density functional theory (DFT), and found that the L_D^S in the BP single crystals was a few hundred nanometers (nm), which is typically larger than the reported measured values for comparable molecular condensates [16,17]. Yost and co-workers have [18] calculated the exciton diffusion lengths of singlet and triplet excitons by using purely ab- initio approaches. Using tetracene as an example, they have examined the fundamental limits of increasing exciton diffusion length and concluded that the only material parameter that could be varied to optimize the singlet exciton diffusion length was the dipole moment. In addition, in their approach regarding triplet excitons, the diffusion coefficient and exciton lifetime could be manipulated independently; hence there was no fundamental limit in increasing the triplet diffusion length. In another study by Terao et al. [19], a virtually linear relationship between the short circuit current (J_{SC}) of a bilayer OSC and the singlet exciton diffusion length L_D^S has been presented. They have calculated the diffusion length in several metal phthalocyanines by generating a line of best fit using the action spectra of the external quantum efficiency in solar cells and deduced that the J_{SC} was correlated with the L_D^S in the metal phthalocyanines. Another development in modeling the exciton diffusion was carried out by Movaghar et al. [20], where Monte Carlo simulation and numerical analytic theory were employed to describe the diffusion and energy relaxation of singlet excitons by Förster resonance energy transfer (FRET). Another studies

[7,21] reported a Monte Carlo simulation of exciton diffusion using random walks based on Förster model for a bilayer OSC by taking into account a constant exciton lifetime.

In all the above theoretical models proposed to study the exciton diffusion dynamics in organic semiconductors, no systematic theoretical analysis has been carried out to elucidate the factors which directly influence the exciton diffusion length L_D, especially for triplet excitons. However, recently, the dependence of L_D on some photophysical parameters of boron subphthalocyanine chloride (SubPc) [22], and triphenylamine (TPA) [23] has been experimentally demonstrated. This paper presents a comprehensive theoretical study of the dependence of L_D in some selected organic solids as a function of the material parameters that govern exciton transfer and how to optimize L_D. Applying the Förster resonance energy transfer (FRET) and Dexter carrier transfer processes for singlet and triplet excitons, we have derived analytical expressions for the L_D and exciton diffusion coefficients (D) as functions of photophysical parameters such as the photoluminescence (PL) quantum yield (ϕ_D), the spectral overlap integral (J), the refractive index (n), the dipole orientation factor (κ^2) and the dipole moment (μ_T). The calculated diffusion lengths in different organic materials are compared with experimental values [14,16,22,24,27-30], and found to be in reasonable agreement. It is expected that this work will add fabrication guidance in selecting the donor acceptor materials for optimal BHJ OSCs.

This paper is structured as follows: the processes involved in the operation of BHJ OSCs are briefly introduced in section 1. In section 2, the theory of both singlet and triplet exciton diffusion to the interface is presented. In section 3, the calculated results for the diffusion lengths and diffusion coefficients for some selected organic materials are presented, and these results are discussed in section 4. Finally, the conclusions drawn are presented in section 5.

Mechanism of Exciton Diffusion

Although several techniques such as spectrally-resolved PL quenching [16,30,34,35], PL surface quenching [17,19,31-33], exciton-exciton annihilation [36-39], bulk quenching with Monte Carlo modelling [40,41] etc., have been employed to measure L_D in organic semiconductors, the results obtained vary from one and another. As a result, there is a growing interest in the basic understanding and accurate determination of the diffusion

length and diffusion coefficient in organic semiconductors. Two general radiationless transfer mechanisms by which excitons can diffuse in organic semiconductors are Förster resonance energy transfer (FRET) and Dexter carrier transfer mechanisms. These mechanisms describe the exciton transfer with respect to the separation distance between the donor and acceptor molecules [42] as shown below.

Förster resonance energy transfer is a singlet-singlet resonance energy transfer, and is suitable for a long-range transfer. In this mechanism, an excited electron in an exciton on a molecule recombines with the hole, rendering the exciton de-excited and its energy is transferred to excite an exciton on a different identical molecule. It is an energy transfer process that takes place between molecules of identical singlet excited states due to dipole-dipole interaction. The rate of transfer k_F of FRET is given by [16,42-45]:

$$k_F = \frac{1}{\tau_H^S} = \frac{1}{\tau_S}\left(\frac{R_F}{R_{DA}}\right)^6,$$
(1)

where R_{DA} is the donor-acceptor (D-A) separation distance, τ_S (τ_H^S) is the lifetime (hopping time) of singlet excitons, and R_F is the Förster radius, given by [43,44]:

$$R_F = \frac{78\times10^{-3}}{\pi}\left(\frac{\kappa^2\phi_D}{n^4}J\right)^{1/6},$$
(2)

where J is the spectral overlap integral, $0 \leq \kappa^2 \leq 4$ is the dipole orientation factor, n is the refractive index of the material and ϕ_D is the PL quantum yield, given by [44,46]:

$$\phi_D = \frac{k_{\mathrm{rad}}}{(k_{\mathrm{rad}} + k_{\mathrm{nonrad}})},$$
(3)

where k_{rad} (k_{nonrad}) is the radiative (non-radiative) decay rate. It may be noted that the rate in Eq. (1) depends on the separation distance as R_{DA}^{-6}.

Substituting Eq. (2) into Eq. (1), k_F is obtained as:

$$k_F = \frac{1}{\tau_H^S} = \frac{1}{\tau_S}\left(\frac{78\times10^{-3}}{\pi}\right)^6\left(\frac{\kappa^2\phi_D J}{n^4}\right)\frac{1}{R_{DA}^6}.$$
(4)

The Dexter carrier transfer mechanism is a close-range transfer process, which involves the transfer of excited electron and hole in an exciton on a molecule to a neighbouring molecule in the ground state. This mostly

occurs when the donor and acceptor separation distance is around 1nm, so there is an overlap of the electronic wavefunctions. This mechanism can be applied to both singlet and triplet excitons but in our calculations we have applied it only to triplet excitons. The triplet exciton transfer rate k_D as a function of R_{DA} is given by [42,45-47]:

$$k_D = \frac{1}{\tau_H^T} = \frac{1}{\tau_T} \exp\left[\frac{2R_D}{d}\left(1 - \frac{R_{DA}}{R_D}\right)\right],$$ (5)

where τ_T (τ_H^T) is the lifetime (hopping time) of triplet excitons, R_D is the Dexter radius, and d is the average length of a molecular orbital. Unlike the inverse sixth-power R_{DA} dependence in FRET [Eq. (4)], the rate of exciton transfer [Eq. (5)] in Dexter's approach decays exponentially with the D-A separation distance [45].

The exciton diffusion coefficient for both singlet (S) and triplet (T) excitons based on Smoluchowski-Einstein mechanism of random walks can be expressed as [48]:

$$D_j = \frac{R_{DA}^2}{6\tau_H^j} = \frac{(L_D^j)^2}{\tau_j},$$ (6)

where $j=S$ or T for singlet or triplet exciton.

Using $k_F = \frac{1}{\tau_H^S}$ in Eq. (6), a relation between Förster transfer rate and the singlet exciton diffusion length L_D^S is obtained as:

$$k_F = \frac{6(L_D^S)^2}{\tau_S R_{DA}^2}.$$ (7)

Using Eqs. (4) and (7) gives an approximate singlet exciton diffusion length as:

$$L_D^S = \frac{48 \times 10^{-6}}{\sqrt{6}\pi R_{DA}^2}\sqrt{\frac{\kappa^2 \phi_D J}{n^4}},$$ (8)

and the corresponding diffusion coefficient is obtained as:

$$D_S = \frac{(L_D^S)^2}{\tau_S}.$$ (9)

Substituting Eq. (8) into Eq. (9) gives:

$$D_S = \frac{3 \times 10^{-10}}{\sqrt{6}\,\pi\tau_S R_{DA}^4}\left(\frac{\kappa^2 \phi_D J}{n^4}\right).$$ (10)

According to Eq. (8), the singlet exciton diffusion length L_D^S depends on the D-A separation distance R_{DA}, the dipole orientation factor κ^2, the quantum yield ϕ_D, Förster's spectral overlap integral J and the index of refraction n.

For Dexter's mechanism, one can obtain the radiative decay rate k_{rad}^T of the triplet from the Einstein A-coefficient of spontaneous emission as [49,50]:

$$k_{rad}^T = \frac{\omega_T^3 \mu_T^2}{3\pi\varepsilon_0 \hbar c^3},$$ (11)

and the inverse of k_{rad}^T gives the radiative lifetime τ_{rad}^T of the triplet as:

$$\tau_{rad}^T = \frac{1}{k_{rad}^T} = \frac{3\pi\varepsilon_0 \hbar^4 c^3}{E_T^3 \mu_T^2}.$$ (12)

The triplet exciton lifetime τ_T is thus obtained from τ_{rad}^T as [45,51]:

$$\tau_T = \tau_{rad}^T \phi_D = \frac{3\hbar^4 c^3}{4k_e E_T^3 \mu_T^2} \phi_D,$$ (13)

where μ_T is the dipole moment for triplet exciton, c is the speed of light, ε_o is the permittivity of free space, $k_e = (4\pi\varepsilon_0)^{-1} = 8.987 \times 10^9$ and $E_T = \hbar\omega_T$ is the triplet exciton energy: $\hbar$ is the reduced Planck's constant and ω_T is the oscillation frequency. According to Eq. (13), the triplet lifetime given depends inversely on the square of the corresponding dipole moment.

Using $k_D = \dfrac{1}{\tau_H^T}$ in Eq. (6) and substituting Eq. (13) into Eq. (6) gives:

$$\frac{k_D R_{DA}^2}{6} = \frac{4k_e E_T^3 \mu_T^2 (L_D^T)^2}{3\hbar^4 c^3 \phi_D}.$$ (14)

Using Eqs. (5) and (14), we obtain an approximate triplet exciton diffusion length as:

$$L_D^T = \frac{\hbar^2}{2\mu_T} \sqrt{\frac{c^3 k_D \phi_D}{2k_e E_T^3}} \left[R_D - \frac{d}{2} \ln(\tau_T k_D) \right],$$ (15)

and the corresponding diffusion coefficient as:

$$D_T = \frac{1}{8\mu_T^2 \tau_T} \left(\frac{\hbar^4 c^3 k_D \phi_D}{k_e E_T^3} \right) \left[R_D - \frac{d}{2} \ln(\tau_T k_D) \right]^2. \qquad (16)$$

We have thus derived the diffusion lengths and diffusion coefficients for singlet [Eqs. (8) and (10)] and triplet [Eqs. (15) and (16)] excitons as functions of the material parameters κ^2, J, n, R_{da}, ϕ_D, τ_T and μ_T. It may be noted that the singlet diffusion length in Eq. (8) does not depend on the singlet exciton lifetime τ_S, and the triplet diffusion length in Eq. (15) does not depend on R_{DA} and the refractive index n of the material.

Results

Table I presents different donor materials with their corresponding input parameters required for calculating the diffusion length L_D^S and diffusion coefficient D_S of singlet excitons. Using Eqs. (8) and (10), and the parameters listed in Table I, we have calculated L_D^S and D_S; these are listed in Table II. The D-A separation distance R_{DA} = 0.45 nm, is used in the calculation for all the materials.

According to Table II, the calculated values of L_D^S for all the chosen materials, with the exception of neat layer of PtOEP range from 5.6 to 66.9 nm, and are found to be in reasonable agreement with the available experimental values, which range from 5.1 to 225 nm [14,16,22,24,27-30] . Although the application of FRET for Nile Red/PCBM has been discussed earlier [57], the diffusion coefficient D_S for this material has not been calculated because the singlet exciton lifetime τ_S is not known. It may be noted that although PTCDA has a longer singlet exciton lifetime, the calculated L_D^S =5.6 nm is smaller than those in all the materials with the exception of PtOEP (see Table II). This is because L_D^S depends directly on ϕ_D and J, and inversely on n [Eq. (8)], and PTCDA has relatively lower ϕ_D, the lowest J and a higher n (Table I). According to Eq. (8), (i) the dependence of singlet diffusion length L_D^S on spectral overlap integral J and PL quantum yield ϕ_D is parabolic, and is therefore expected to be similar, as it can be seen from Figs. 1 and 2 and (ii) L_D^S increases as the refractive index n decreases (not shown here).

8

Using Eq. (8), the diffusion length of singlet excitons L_D^S is plotted as a function of the spectral overlap integral J in Fig. 1 for all the materials listed in Table I, excluding SubPc and pure PtOEP. This is because SubPc has the lowest value at all J, and PtOEP has similar behaviour as CBP:10% PtOEP. As seen in Fig. 1, Nile Red/PCBM has the highest L_D^S followed by CBP and CBP:10% PtOEP at all values of J.

Using Eq. (8), the L_D^S is also plotted as a function of the PL quantum yield ϕ_D in Fig. 2 for all the materials listed in Table I, excluding PTCDA and PtOEP. This is because PTCDA has the lowest value at all values of ϕ_D, and PtOEP has similar behaviour as CBP:10% PtOEP. Fig. 2 shows that for $\phi_D = 1$, DIP (upright) has the highest L_D^S followed by CBP:10% PtOEP.

Table III presents different donor materials with their corresponding input parameters required for calculating the diffusion length L_D^T and diffusion coefficient D_T of triplet excitons. Using Eqs. (15) and (16), and parameters listed in Table III, we have calculated L_D^T and D_T; these are listed in Table IV.

The D-A separation distance $R_{DA} = 0.45$ nm, is used in the calculation for all the materials. Following [42], the average length of a molecular orbital $d = 0.11$ nm found in Ir(ppy)₃:PMMA is assumed in our simulation for all triplet materials.

We find the calculated $L_D^T = 42.5$ nm for Ir(ppy)₃:PMMA, which is comparable to the diffusion lengths in several organic materials, such as PtOEP ($L_D^T = 30$ nm) [25, 26], [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) ($L_D^T = 21$ nm) [25], polyfluorene (F8-F6) ($L_D^T = 50$nm) [59], poly(9,9′-di-n-octylfluorene-ran-N,N′-bis(4-n-butylphenyl)-N,N′-diphenyl-1,4-benzenediamine) (F8-PDA) ($L_D^T = 41$ nm) [58], polycations bearing tris(2,2¢-bipyridine)ruthenium(II) (Ru) moieties (P(CM-Rux)) ($L_D^T = 36$ nm) [59] and palladium tetrakis(4-carboxyphenyl)porphyrin (PdTPPc) ($L_D^T = 30$ nm) [60]. There are no measured values of L_D^T for Ir(ppy)₃:PMMA reported in the literature, however the application of close-range Dexter carrier transfer mechanism for this

material has been discussed [42]. According to Table IV, the calculated values of L_D^T = 1.75 nm [Eq. (15)] and

D_T = 0.0038 nm²s⁻¹ [Eq. (16)] in PtOEP are much shorter than the corresponding measured values given in Table

IV; this may be attributed to the much lower value of ϕ_D =0.001(Table III), used in the calculations. However,

L_D^T =1.75 nm agrees very well with a related triplet material (Ir(ppy)₃-cored dendrimers) with L_D^T =2 nm [61].

The smaller L_D^T in neat layer PtOEP implies that the diffusion length of triplets may be comparable to that of

singlets in fluorescent materials.

Using Eq. (15), the diffusion length of triplet excitons L_D^T is plotted as a function of the dipole moment μ_T

in Fig.3 for Ir(ppy)₃:PMMA and PtOEP. Fig. 3 illustrates that the triplet diffusion length increases as the dipole

moment decreases, as it is obvious from Eq. (15) and here again the diffusion length in Ir(ppy)₃:PMMA is much

higher than that in pure PtOEP at all μ_T .

Using Eq. (15), the L_D^T is plotted as a function of the PL quantum yield ϕ_D in Fig. 4 for Ir(ppy)₃: PMMA

and PtOEP, which illustrates that the diffusion length increases with the PL quantum yield ϕ_D .

According to these results shown in Figs. 1-4, it may be deduced that if one can vary the photophysical

parameters such as spectral overlap integral, PL quantum yield, refractive index and dipole moment of the organic

active layer by incorporating other host materials [22,23,51,62], one can increase the singlet and triplet exciton

diffusion lengths. Therefore, present results may be expected to be very useful in manipulating these parameters

with a view to improve the performance of BHJ OSCs.

Discussions

A comprehensive study of diffusion lengths, diffusion coefficients, lifetimes of excitons in organic solids has

been carried out. The above results suggest the following: 1) the singlet exciton diffusion length L_D^S can be

increased by; (i) increasing the PL quantum yield ϕ_D ; (ii) increasing the spectral overlap integral J and (iii)

decreasing the refractive index n of the material, and 2) the triplet exciton diffusion length L_D^T can be enhanced

by increasing the PL quantum yield ϕ_D and reducing the dipole moment μ_T . These may be achieved through

doping the organic solids into broad-optical-energy-gap host materials like CBP, tris(8-hydroxyquinoline)-aluminium (III) (Alq$_3$), p-bis(triphenylsilyl)benzene (UGH2) , m-bis(triphenylsilyl)benzene (UGH3), 9,9'-spirobisilaanthracene (UGH4), N,N'-diphenyl-N,N'-bis(3-methylphenyl)-1,1-biphenyl-4,4'-diamine (TPD) and 2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline (BCP) [22,23,51,62]. This is in direct contrast with previous studies [5-10], where the L_D was found to decrease with increasing dopant concentrations due to an increase in D-A separation distance R_{DA}. In addition, the calculated L_D values for the various organic materials in Tables (II) and (IV) are found to be comparable with the diffusion lengths in several organic solids (small molecular donor, polymer donor materials, and acceptor materials) [64-78].

A commonly used hole transporting material-NPD in organic light emitting diodes (OLEDs), has been used as a donor material in OSCs [16,63]. According to Table II, we obtain L_D^S =13.8 nm in NPD, which is comparable to the diffusion length in organic solids, such as poly[3,4-dihexyl thiophene-2,2':5,6'-benzo[1,2-b:4,5-b']dithiophene] (PDHBDT) (L_D^S =13) [64], poly(9,9-dioctylfluorene-2,7-diyl-co-benzothiadiazole) (PFBT) (L_D^S =12) [65] and ladder-type poly(p-phenylene) (LPPP) (L_D^S =14) [66]. Similarly, the calculated L_D^S =5.6 nm in PTCDA and 6.8 nm in SubPc are comparable to the measured values in PTCDA (L_D^S =7 nm) [30], SubPc (L_D^S =7.7 nm) [20] and dicyanovinyl-terthiophene (DCV3T) (L_D^S =5.6 nm) [67]. Small diffusion lengths have also been measured for polymer donor materials such as polyphenylene-vinylene (PPV) (L_D^S =7nm) [68], poly (3-(4'-(1'',4'',7''-trioxaoctyl)phenyl)thiophene) (POEPT) (L_D^S =5.0 nm) [69], and poly(3-hexylthiophene) (P3HT) (L_D^S = 4.8 nm [70]; ~5.3 nm [70] and ~4 nm [71]).

For DIP-(flat), we obtain L_D^S =9.9 nm, which is comparable to the diffusion length in materials like blue-emitting 4,4'4,4'-bis(2,2'2,2'-diphenylvinyl)-1,1'1,1'-biphenyl (DPVBi) (L_D^S =8.7 nm) [72], poly(2,5-bis(3-hexadecylthiophen-2-yl)thieno[3,2-b]thiophene) (PBTTT) (L_D^S =10) [73], P3HT (L_D^S = 9 nm) [70], copper phthalocyanine-CuPc (L_D^S =10 nm) [74], and Ni-phthalocyanine (NiPc) (L_D^S =9.1 nm) [19]. Also we obtain L_D^S = 16.1 nm in DIP-(upright), which is comparable to its experimental value (L_D^S =16 nm) [16], and the L_D^S =15 nm in tetrabenzoporphyrin (BP) [75]. These values are in contrast with the measured values reported by Topczak et al. (L_D^S =60 nm) [24], and Kurrle and Pflaum (L_D^S =80-100 nm) [14]. The difference in calculated L_D^S

between DIP-(flat) and DIP-(upright) is mainly attributed to the difference in their dipole orientation factors (κ^2) (see Table I).

Although, the measured singlet exciton diffusion length for Nile Red/PCBM is not known, its calculated value (L_D^S=39.2 nm) in Table II is comparable to the singlet exciton diffusion length in some organic materials such as buckminsterfullerene-C_{60} (L_D^S=40 nm) [74] and zinc phthalocyanine-ZnPc (L_D^S=30 nm) [76].

For neat layer PtOEP, we obtain L_D^S=0.69 nm, which is considerably smaller than its measured value [16]; this may be due to the substantially lower PL quantum yield ϕ_D and spectral overlap integral J used in the calculation, and it is clearly the shortest diffusion length in the organic materials studied herein. However, L_D^S =0.69 nm agrees reasonably with L_D^S=0.7 nm in meso-tetraphenylporphyrin (TPP) [78], L_D^S=1 nm in triphenylamine-cored compounds (TPA-cored materials) [23], L_D^S=1 nm in Fe-phthalocyanine (FePc) [19], L_D^S =1.4 nm in co-phthalocyanine (CoPc) [19], and L_D^S=2 nm in copper tetrabenzoporphyrin (CuPc) [75].

In view of the various experimental results presented herein, it is obvious that different experimental techniques reveal somewhat different diffusion lengths. For example, the technique used to measure the diffusion lengths in DIP-(upright) by Topczak et al. (L_D^S=60 nm) [24] and Kurrle and Pflaum (L_D^S=80-100 nm) [14] is known to give overestimated values [16]. The discrepancies in the experimental values may also be attributed to neglecting the radiationless transfer from the donor to the quenching layer [16,70]. In addition, the discrepancies may also occur due to the varying magnitude of the crystallinity in different samples [16]. Mostly, the organic materials with higher degree of crystallinity exhibit longer exciton diffusion length L_D^S. For instance, the L_D^S of PTCDA has been measured by Lunt et al. [16], using spectrally resolved PL quenching, where they observed an increase in L_D^S from 6 to 20 nm as the average diameter of crystalline medium increases from 100 to 400 nm. Yang et al. [78] have measured the singlet exciton diffusion length of ZnPc films with different level of crystallinity and observed an increase in L_D^S from 9 to 16 nm. Rim et al. [31] have demonstrated that a more ordered trans-isomer has L_D^S=5 nm compared to a disordered cis-isomer with L_D^S=2.6 nm in perylene derivative. The L_D^S of P3HT has been measured by Sim et al. [79], using spectrally-resolved PL quenching in bi-layer OSCs as a function of annealing temperature and observed an increase in L_D^S from 3.3 to 7 nm with the annealing

temperature, which results in an increase in the level of crystallinity. However, it has been proven that processing organic solids with high boiling point supplement can lead to a decrease of L_D^S, despite a concomitant increase in the level of crystallinity [80].

Triplet excitons are known to possess longer L_D^T than singlet excitons owing to their much longer lifetime τ_T [see Eq. (6)]. However, L_D^T values ranging from 10-20 nm have been measured recently, which are comparable to the diffusion length of singlet excitons L_D^S [16,60,81-84]. On the contrary, several studies have reported L_D^T values of more than 100 nm [85-89]. Furthermore, different L_D^T values varying from 10-250 nm have been reported for the same materials [82,85,90-92]. As stated above, such discrepancies in the experimental values may be attributed to the different techniques used to measure the diffusion length. Phosphorescence quenching has therefore been recommended as the only simple method suitable for measuring the L_D^T in phosphorescent materials [16,93].

To elucidate the factors which directly influence the exciton diffusion length, we perform a few simulations by varying the different photophysical parameters. According to Figs. 1 and 2, if the spectral overlap integral J and PL quantum yield ϕ_D can be increased to compensate the increase in R_{DA} with dilution or doping [22,23,51,62], the exciton diffusion length can still be increased or kept constant. For example, the exciton diffusion length in pure SubPc and mixed with UGH2 to increase R_{DA} has been measured by Menke et al. [22], where they observed that mixing of 25 wt% SubPc in the host material (UGH2) resulted in an increase in L_D^S from 10.7 to 15.4 nm. Although, by increasing R_{DA} in SubPc by mixing it with UGH2, according to Eq. (8), one expects a decrease in L_D^S; the increase in the diffusion length was attributed to increase in J and ϕ_D, and decrease in n. Here, the increase in ϕ_D is due to a decrease in non-radiative decay rate (k_{nonrad}) [Eq. (3)]. Similarly, J increased due to a reduction of the Stokes-shift in SubPc fluorescence. It was also observed that the reduction in n was attributed to the low relative permittivity of UGH2 [22]. Rasys et al. [20] have measured the exciton diffusion length in triphenylamine (TPA)-based amorphous films upon blending them with phenylethenyl side-arms. The resulting increase in the number of phenylethenyl side-arms resulted in an increase in L_D^S from 1 to 7 nm. This increase was due to an increase of J, which is attributed to a decrease in Stokes-shift [23]. In

another study [62], it has been reported that Ir(ppy)$_3$ has a higher ϕ_D of 0.97 $\pm$ 0.02 when doped in the large optical energy gap host, CBP. A similar result was observed [51], where 8.4 wt% PtOEP was doped into CBP host to increase ϕ_D from 0.001 to 0.37 and the corresponding triplet lifetime τ_T increased from 0.10 μs to 30 μs [Eq. (13)].

In a previous work [26], a neat layer of PtOEP was used as donor in association with the electron acceptor C$_{60}$ to form a multilayer heterojunction cell (ITO/PEDOT/PtOEP/C$_{60}$/BCP/Al) and the measured ϕ_D was found to be very low (see Table III). Generally, Förster mechanism is applied to only singlet excitons; however, a triplet exciton that is located at a phosphorescent donor can also undergo long-range Förster resonance energy transfer [94-99]. By doping 10 wt% PtOEP into CBP host [29], ϕ_D and J have increased due to the increase in the spin-orbit interaction [99] . The significantly large spectral overlap of CBP:10% PtOEP (J = 1.9$\times$10^{14} M^{-1}cm^{-1}nm^4) implies that PtOEP has the tendency of undergoing FRET [19], although PtOEP is often considered as a triplet state that undergoes close-range Dexter carrier transfer [30]. As a result, doping PtOEP into CBP increases L_D^S of PtOEP from 0.69 to 66.9 nm (Table II). The large calculated L_D^S =66.9 nm compared to its corresponding smaller measured value L_D^S =5.1 nm may be as a result of the higher J .

According to Fig. 3, one may increase the triplet exciton diffusion length in organic semiconductors by decreasing the dipole moment μ_T, which in accordance with Eq. (13) means choosing organic materials or blended-organic materials with longer exciton lifetimes, and higher exciton mobility. It is established that the lifetime of triplet excitons is about three orders of magnitude greater than that of singlet excitons [100-102]. For instance, τ_T = 1.33 μs of Ir(ppy)$_3$:PMMA is longer than any singlet exciton lifetime. Also, comparing L_D^T =1.75 nm and L_D^S =0.69 nm in PtOEP (Tables II and IV), it is obvious that diffusion length in triplet excitons is higher than the diffusion length in singlet excitons. As shown in Fig. 3, at μ_T = 5.0$\times$10^{-22} eV$^{1/2}$m$^{3/2}$, for Ir(ppy)$_3$:PMMA we have obtained L_D^T = 382.1 nm, which is much higher than that observed experimentally. An exciton with a longer diffusion length has a higher probability of reaching the D-A interface before recombination. As a triplet exciton has higher diffusion length, one may be tempted to generate more triplet excitons in a BHJ OSC. However, it may also be kept in mind that the binding energy of triplet excitons (E_B^T) is much higher and hence they are difficult to dissociate unless one can find pairs of donor and acceptor materials with their LUMO offsets more

than or equal to the triplet exciton binding energy [103,104]. These results may be expected to develop new organic materials (especially donor materials) which can further improve the performance of BHJ OSCs.

Conclusions

In summary, we have derived expressions for singlet and triplet exciton diffusion lengths and diffusion coefficients using Föster resonance energy transfer and Dexter carrier transfer mechanisms, respectively, for BHJ OSCs. The calculated diffusion lengths for the selected materials are comparable with the experimental values, with the exception of neat layer of PtOEP, which has its calculated L_D far below the experimental values. The dependence of singlet and triplet diffusion lengths on the spectral overlap integral J, PL quantum yield ϕ_D, refractive index n and dipole moment μ_T has been analyzed theoretically. It is found that by varying J, ϕ_D and n, upon diluting the organic solid in a host material, one can increase the singlet exciton diffusion length L_D^S, despite an increase in R_{DA}. Likewise, triplet exciton diffusion length L_D^T can be increased by increasing ϕ_D upon doping, or by decreasing μ_T. This implies that several organic solids with different morphologies and functions can be blended to optimize the performance of BHJ OSCs.

Conflict of Interest

The authors declare that they have no conflict of interest.

Acknowledgement

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Figure Captions

Fig. 1. Singlet exciton diffusion length L_D^S in various organic materials plotted as a function of spectral overlap integral J.

Fig. 2. Singlet exciton diffusion length L_D^S in various organic materials plotted as a function of PL quantum yield ϕ_D.

Fig. 3. Triplet exciton diffusion length L_D^T in Ir(ppy)$_3$:PMMA and PtOEP plotted as a function of dipole moment μ_T.

Fig. 4. Triplet exciton diffusion length L_D^T in Ir(ppy)$_3$:PMMA and PtOEP plotted as a function of PL quantum yield ϕ_D.

Table Captions

Table I. Input parameters required for calculating L_D^S (Eq. (8)) and D_S (Eq. (10)) for singlet excitons in NPD, CBP, SubPc, PTCDA, DIP, CBP:10% PtOEP, and Nile Red/PCBM.

Table II. Calculated diffusion length (L_D^S calc.) from Eq. (8), diffusion coefficient (D_S calc.) from Eq. (10) and measured diffusion length (L_D^S meas.) of singlet excitons in NPD, CBP, SubPc, PTCDA, DIP, CBP:10% PtOEP, and Nile Red/PCBM using input parameters in Table I.

Table III. Input parameters required for calculating L_D^T (Eq. (15)) and D_T (Eq. (16)) for triplet excitons in Ir(ppy)₃ and PtOEP

Table IV. Calculated diffusion length (L_D^T calc.) from Eq. (15), diffusion coefficient (D_T calc.) from Eq. (16) and measured diffusion length (L_D^T meas.) of triplet excitons in Ir(ppy)₃:PMMA and PtOEP using input parameters in Table III.