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Influence of Photophysical Parameters of Photoactive Materials on Exciton Diffusion Length and Diffusion Coefficient in Bulk Heterojunction Organic Solar Cells

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Abstract : It has been experimentally demonstrated that exciton diffusion length in organic solids can be improved by fine-tuning the material parameters that govern exciton transfer. Here, a theoretical study is carried out to support this finding. We have therefore derived expressions for the exciton diffusion length and diffusion coefficient of singlet and triplet excitons using Förster resonance energy transfer and Dexter carrier transfer mechanisms and are plotted as a function of photoluminescence (PL) quantum yield, spectral overlap integral, refractive index and dipole moment of the photoactive material. We found that singlet exciton diffusion length increases with PL quantum yield and spectral overlap integral, and decreases with increase in refractive index. Likewise, the triplet exciton diffusion length increases when PL quantum yield increases and dipole moment decreases. The calculated diffusion lengths in different organic materials are compared with existing experimental values and found to be in reasonable agreement. The results are expected to provide insight in developing new organic materials for fabricating bulk heterojunction (BHJ) organic solar cells (OSCs) with better photoconversion efficiency.

Keywords : Dexter carrier transfer, diffusion coefficient, exciton diffusion length, Föster resonance energy transfer, photoactive materials, photophysical parameters
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