Optimization and Understanding of Exciton Diffusion in Organic Solar Cells via Novel Monte Carlo Modeling

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Organic photovoltaics are at the forefront of renewable energy because of cheap cost, nontoxicity, scalability, and rising efficiencies. However, PCBM (phenyl- C61-butyric-acid methyl ester) electron acceptor material aggregates in certain synthetic compounds, thereby decreasing relative quenching efficiency (Q), exciton diffusion length (LD), ultimately lowering the performance of molecular electronics.The singlet exciton diffusion properties of two porphyrin molecules, tetrakis(4-carbomethoxyphenyl) (TCM4PP) and tetrakis(4-carbooctoxyphenyl) (TCO4PP) were explored in conjunction with PCBM for use in solar energy conversion applications.The exciton diffusion coefficient (D) and the exciton diffusion length (LD) for each porphyrin derivative were obtained by modeling the quenching efficiency and PL lifetime decay data using a 3D exciton Monte Carlo diffusion simulation. It is determined that the lower the volume fraction of PCBM, the higher the accuracy of exciton diffusion length, and the less the aggregation. Singlet exciton diffusion lengths for TCM4PP of volume fractions of 0.06, 0.20, and 0.23 were respectively determined to be 15.133 nm, 12.327 nm, and 9.39 nm. Exciton diffusion lengths for TCO4PP at volume fractions of 0.028, 0.03, 0.084, and 0.2 were determined to be 34.508 nm, 33.853 nm, 17.808 nm, and 12.342 nm-almost twice the exciton diffusion length of TCM4PP. Single exponential lifetime decays and diffusion lengths indicate that longer alkyl chains enhance photocurrent conversion efficiency in comparison between octyl and methyl groups, making more efficient organic solar cells.