Improving Exciton Transport in Novel Tetracarboalkoxyphenyl Porphyrin Thin Films for Enhanced Organic Optoelectronics

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Currently, optoelectronic devices such as solar cells, photodetectors, and light emitting diodes are plagued by inefficiencies, toxicity, and cost. Porphyrin thin films have recently shown potential as alternative light-harvesting systems because of their broad and tunable absorption spectrum. However, the performance of existing porphyrin-based systems is far below optimal. In particular, aggregation in porphyrin thin films, disordered self assembly, and shorter-than-optimal exciton diffusion lengths significantly hinder energy transfer and subsequently prevent integration into organic electronic devices. In this study, I greatly enhanced performance by introducing long alkyl chain substituents to improve thin-film organization. First, three novel tetracarboalkoxyphenyl porphyrins (TCAPPs) with varying substituent chain lengths were designed and analyzed using Density Functional Theory. Next, I synthesized the TCAPPs and spectroscopically examined their excited-state energy transfer dynamics. My results indicated that longer alkyl chains increase order in the arrangement of TCAPPs within thin films, allowing for longer exciton diffusion lengths and improved quenching of excited states. In particular, I observed a notable increase in exciton diffusion length from 15 nm for the methyl-substituted control TCAPP to 28 nm for the octyl-substituted TCAPP, which is nearly unprecedented in porphyrin thin films. My findings are a significant advance toward the development of structure-property relationships at the molecular level and incorporation of porphyrins into efficient organic optoelectronics.