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The Influence of Molecular Geometry on Photophysical Properties and Self-Assembly of Phthalimide End-Capped Thiophene-Based Organic Molecules

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Abstract

The synthesis of π -conjugated organic small molecules with n-octyl substituted thiophene phthalimide end-capping units have been reported. A combination of absorption and emission spectroscopy, cyclic voltammetry, ultraviolet photoelectron spectroscopy, density functional theory calculations and atomic force spectroscopy were used to elucidate the impact of molecular dimensionality on photophysical properties and self-assembly.

Keywords: small organic molecule; organic photovoltaics; phthalimide end-capped oligothiophene; bulk heterojunction; self-assembly

Introduction

Organic π -conjugated materials offer a platform for a broad range of optical and electronic applications such as light-emitting diodes, organic photovoltaics, and organic field-effect transistors.¹⁻⁶ This is mainly attributed to their optoelectronic characteristics, low fabrication costs and ease of processing.⁷⁻⁹

Key geometries of organic semiconductors realized by researchers are propeller or pin-wheel architectures (often referred as star-shaped)^{10–14} and non-planar, dimeric scaffolds.^{15–17} These architectures showed superior solar cell performance over planar structures due to their tendency

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