Solid State Packing Control in Materials for Solar Cells

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Abstract

Diketopyrrolopyrroles (DPPs) are promising building blocks for organic electronics in general due to their optical properties, good thermal and photochemical stability, good electron affinity for tuning the frontier energy levels, and excellent planarity for enhancing intermolecular interactions and increasing charge carrier mobility.1 DPPs have huge chemical versatility2 which makes them easy to incorporate in various materials or to be exploited as small molecules for molecular and supramolecular materials, and consequently used for photovoltaic applications.3

This work presents thiophene based DPP chromophores whose structure and stereochemistry are defined to ensure high specificity in intermolecular interactions in the solid state (Figure 1). These specific functions are addressed through the nitrogen atom and the aromatic rings of the DPP core to control the solubility of the molecule and the packing of the material, and ultimately improve the electron transport and charge collection. Insights of the electronic properties of those chromophores were obtained by solution and solid absorption spectroscopy, cyclic voltammetry and spectroelectrochemistry. Studies in solid state *via* single crystal X-ray diffraction shows unique organisation of the molecules driven by intermolecular hydrogen bonding, as well as important changes in the geometry of the molecule due to other intra- and inter-molecular interactions.

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References:

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