

Organic Semiconducting Nanostructures Via Conjugated Polymer Self-Assembly

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It is well known that the arrangement of conjugated polymer or oligomer molecules in the solid state has a major influence on the absorption, luminescence, and charge transport properties. This comes as a consequence of the π - π interactions between conjugated segments on adjacent chains. Here we illustrate how those intermolecular interactions can be controlled by modifying the molecular architecture and the chain assembly in the solid state. For this study, we combine theoretical modeling of chain assembly, as investigated with force-field molecular mechanics and dynamics, and the experimental observation of the thin film microstructure and local electrical properties with Atomic Force Microscopy. We show how the formation of fibrillar structures can be controlled via the one-dimensional assembly of conjugated segments via π -stacking. The relationships between the polymer chain assembly, the microscopic morphology and the optoelectronic properties are illustrated for field-effect transistors and photovoltaic devices. The interest of incorporating carbon nanotubes in the active layers of solar cells (see figure below) is also evaluated.

