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Morphological investigations of naphthalene diimide derivatives

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Solution-cast, organic field-effect transistors (OFET) have many advantages, such as rapid, large area fabrication, low production cost and flexible substrates making them ideal for specialized application such as flexible displays and radio frequency identification.

The small molecule organic semiconductor (OSC) naphthalene diimide (NDI) provides a versatile framework with which to build upon and explore the effects of chemical functionalisation.

Over the past year, we have utilized two complimentary synchrotron based techniques to examine the effect on structure and morphology as the basic NDI framework is functionalised.

At the soft x-ray beamline, Near Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy allowed us to explore the surface molecular orientation and electronic changes. Expansion of the NDI core was found to give higher average tilt angles with core-expanded derivatives also maintaining their high average tilt angle when annealed.

At the SAXS/WAXS beamline these same materials were investigated using Grazing Incidence Wide Angle X-ray Scattering (GIWAXS) to assess crystallinity and molecular packing. The data confirms both the highly edge on packing behaviour of the core expanded set and the drastic change to the molecular unit cell upon NDI core expansion. The – stacking distance of the conjugated cores, which is an important element of transistor design to allow effective charge transfer, is also measured for each of the materials.

This information will aid and inform the ongoing design of our NDI molecules as we progress towards a high mobility, air stable OFET.

Keywords or phrases (comma separated)

Small molecule, organic semiconductor, OFET, n-type

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