STRUCTURE FORMATION AND ALIGNMENT OF POLYMER SEMICONDUCTORS IN THIN FILMS

Mukundan Thelakkat[a], Christian Müller[a], Christopher R. McNeill[b] and Eliot Gann[b]

[a]Applied Functional Polymers, Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany
[b]Department of Materials Science and Engineering, Monash University, Wellington Road, Clayton, Victoria, 3149, Australia

In thin films of semiconductor polymers, the polymer chains typically exhibit distinct orientation with respect to the substrate. The planar pi-face of the backbone can orient either in edge-on or face-on manner. Especially, an edge-on alignment is favorable for transport in thin film transistors, whereas face-on alignment is considered to improve vertical transport as desired in solar cells. However, molecular orientation is among the very few parameters that usually cannot be controlled when tailoring new semiconducting polymers. Here we show that both the mode of orientation as well as the degree of alignment can be well controlled by exploiting diffusive non-covalent interactions along the backbone using polydiketopyrrolopyrroles (PDPPs) as a case study.

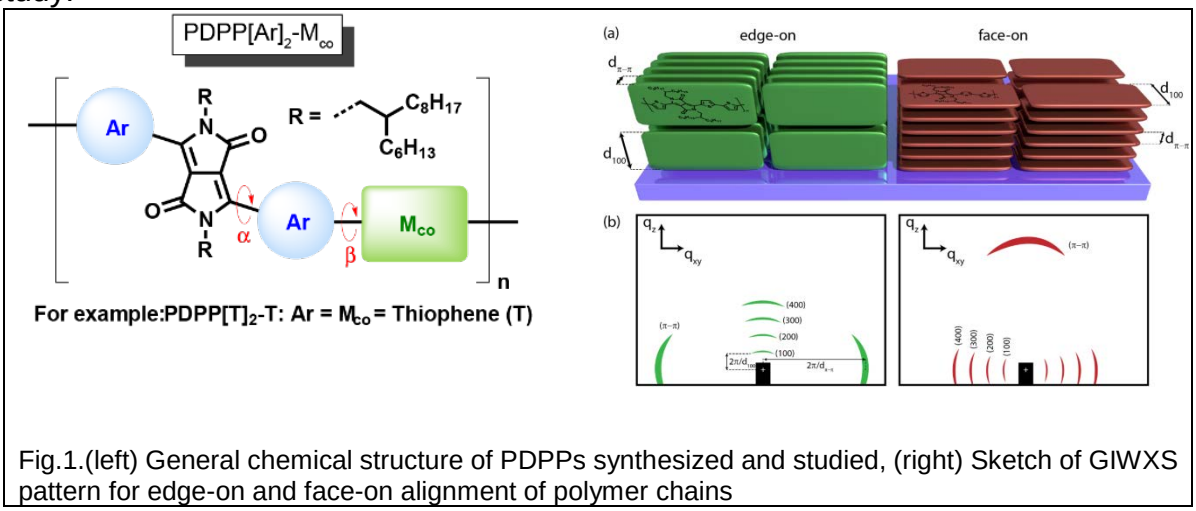

Fig.1.(left) General chemical structure of PDPPs synthesized and studied, (right) Sketch of GIWXS pattern for edge-on and face-on alignment of polymer chains

By strategically varying the chemical structure in a systematic way, we attribute for the first time, the precise control of orientation based on diffusive non-covalent interactions. Our results demonstrate how orientation in thin films of semiconducting polymers can be controlled and optimized by rational design. This study enables high-performance organic semiconductors with the additional benefit of tailored orientation that fits the desired application.

Keywords: Charge transport; Polydiketopyrrolopyrroles, molecular orientation, GIWAXS, conjugated polymers

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