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Key role of structural order and in-plane alignment on optical and charge transport properties of organic (semi)-conductors

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This presentation focuses on recent advances in growth control and oriented crystallization of (semi)-conducting materials for organic electronic applications. The performance and lifetime of organic electronic devices are critically dependent on the morphology of the active layers and structural order of the materials. For instance both molecular and crystalline orientations of polymer semiconductors determine optical and charge transport properties in thin films since these properties are by essence highly anisotropic.

Particular emphasis will be given to the progress made in high-temperature rubbing of conjugated polymers and molecular systems films. This effective large scale alignment method can orient a large palette of semiconductors with *n*- or *p*-type character without the use of alignment substrate.[1] High degrees of crystallinity and in-plane alignment can be obtained which provide well-defined electron diffraction patterns essential for structure refinement. The concurrent roles of the polymer molecular weight distribution and the rubbing temperature (T_R) on the in-plane orientation have been rationalized for P3HT and PBTTT.[2a] Correlations are drawn between nanomorphology/crystallinity on one side and charge transport and optical properties on the other side. It is shown that the exciton bandwidth in P3HT crystals is determined by the length of the average planarized chain segments in the crystals. The high alignment and crystallinity observed for T_R > 200 °C cannot translate to high hole mobilities parallel to the rubbing because of the adverse effect of amorphous interlamellar zones interrupting charge transport between crystalline lamellae of semi-crystalline P3HT.[2b] As opposite, hole mobilities along the polymer chains of rubbed PTB7 films are observed to be 6 times higher than the non-rubbed films.[3] This is due to the smectic- like character of this alternated donor-acceptor copolymer. Interestingly high-Tr rubbing and post annealing process of PTB7 provide well-defined electron diffraction pattern. Combined with DFT calculation, this helps refining the structure and the chain conformation of this benchmark electron donor polymer for OPV.

In a second part of this presentation, we show that soft doping of aligned P3HT yields highly oriented conducting polymer films with anisotropic charges and thermal conductivities. The thermoelectric properties are enhanced along the rubbing direction. The unique in-plane orientation in such conducting polymer films helps rationalizing the mechanism of redox doping.[4]

Références

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