experimental (XRD, grazing incident beam X-ray scattering, neutron diffraction) and computational (molecular dynamics, artificial intelligence) techniques mutually inspire one another and allow developing and verifying a structural model of a polymer system. Each of the contributing pieces listed above by themselves are not enough to develop a good structural model, while combining insight into the studied problem provided by each of them leads to one which is reliable.

References:

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Combination of GIWAXS and TEM study in understanding polymer-fullerene fibrillar network structure

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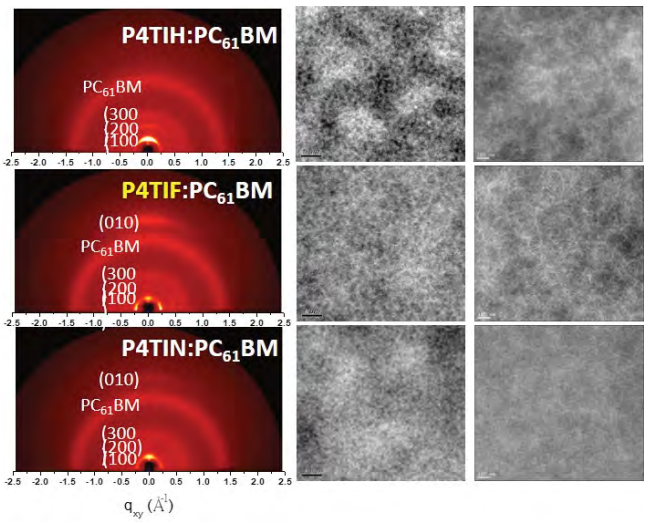
In addition to the larger absorption coefficient and longer absorption wavelength, high short-circuit current density can be associated to the high portion of face-on, in-plane crystallite orientation of **P4TIF**, which is evident by GIWAXS study. GIWAXS study reveals that the face-on (in plane) orientation is most pronounced, lamellar structure, (100), pi-pi stacking structure, (010), and crystallite correlation length are more significant or longer than those of **P4TIN**. Moreover, thin film morphology probed by TEM reveals the fibril network nanostructure, which is more pronounced in $PC_{61}BM$-blended **P4TIF** thin films than **P4TIN** ones. The chemical structure difference between **P4TIF** and **P4TIN** is the fluorine (F) and nitrile (CN) substituent. Such difference in fibrillary morphology, which is in turn due to the different molecular interaction of F or CN, promotes the photocurrent output and hence short-circuit current density of the polymer-based organic photovoltaics.



Keywords: GIWAXS, TEM, polymer-fullerene fibril