

Abstract Submitted
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Orientation and Order in High-Efficiency Polymer Solar Cell Active Layers M.R. HAMMOND, R.J. KLINE, L.J. RICHTER, C.L. SOLES, D.M. DELONGCHAMP, NIST, T. XU, L. YU, Univ. Chicago, M.F. TONEY, SSRL — Using a combination of scattering and spectroscopy techniques, we have characterized molecular orientation and order in bulk heterojunction (BHJ) organic photovoltaic cells based upon thieno[3,4-*b*]thiophene-*alt*-benzodithiophene copolymers (PTB) and fullerene derivatives. The various techniques probe complimentary aspects of the full distribution of (e.g.) polymer chain orientations, so analysis of the data in tandem allows us to evaluate the relative likelihood of several model distributions. Specifically, X-ray diffraction data yielded a full orientation distribution for the polymer pi-stacking direction within well-ordered regions, with the nominal result of a strong preference for pi-stacking in the vertical direction. This structural characteristic may enhance vertical charge mobility and thus be one factor leading to the outstanding performance of PTB based devices. However, the most plausible model distribution would suggest that those ordered (diffracting) regions of the PTB BHJ films comprise only a small percentage of the total polymer volume within the film.

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