Correlated molecular orientation in all-polymer solar cells and its role in free charge generation

BRIAN A. COLLINS, NIST, MARCEL SCHUBERT, STEFFEN ROLAND, RICCARDO DI PIETRO, ROBBERT STEYRLEUTHNER, University of Potsdam, KOEN VANDEWAL, ALBERTO SALLEO, Stanford University, WOLFRAM SCHINDLER, KONSTANTINOS FOSTITROPOULOS, Helmholtz-Zentrum Berlin, ZHIHUA CHEN, ANTONIO FACCHETTI, Polyera Corporation, HARALD ADE, NCSU, DEAN DELONGCHAMP, NIST, DIETER NEHER, University of Potsdam — New polymers with high electron mobilities have spurred research in organic solar cells using polymer rather than fullerene acceptors due to their potential of increased diversity, stability and scalability. However, all-polymer solar cells have thus far struggled to keep up with their polymer-fullerene counterparts. We examine this issue by investigating the effect of additives on morphology correlated to optoelectronic properties within poly(3-hexylthiphene), P(NDI2OD-T2) blend devices. Resonant X-ray microscopy and scattering along with energy-filtered electron microscopy monitor the evolution of domain size and purity, while X-ray diffraction and a novel polarized X-ray scattering technique reveal a reorientation of the molecules with respect to the donor-acceptor interface, correlating well with device photocurrent. In addition, low efficiency in separating directly excited charge transfer states ties the low device efficiency to geminate recombination. Thus, anisotropic polymer electronic orbitals may necessitate correlated donor-acceptor molecular orientation for efficient charge generation and represent an extra hurdle compared with the isotropic fullerene in realizing efficient devices.

Brian Collins
NIST - Natl Inst of Stds Tech

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