Harnessing the Power of Molecular Dynamics: A Nanoscale View of Organic Photovoltaic Materials

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Abstract: We utilized virtual site coarse-grained molecular dynamics to accurately model nanoscale systems of large, complex materials used to make organic photovoltaics. Our system consisted of two semi-conductors: an electron-donating polymer and an electron-accepting non-fullerene molecule.

In neat film simulations, the donor polymer remained amorphous, while the non-fullerene acceptor molecule assembled into highly ordered structures. We extract scattering profiles for these materials using Fast Fourier Transform. Starting from intimately mixed blend of the two materials, we show the acceptor and donor phase separated into distinct domains. When blend simulations started from a completely segregated state, the non-fullerene molecule first penetrated the polymer donor domain, followed by polymer chain swelling, resulting in a mixed phase interface.

Our method still preserves molecular details, and we capture these details by calculating the fraction of π-stacked conjugated rings between donor and donor, acceptor and donor, and acceptor and acceptor. Atomistic details within polymer mixtures and interfaces are of interest to many fields in polymer science, and our research demonstrates the capabilities of virtual site coarse graining to study their morphology.