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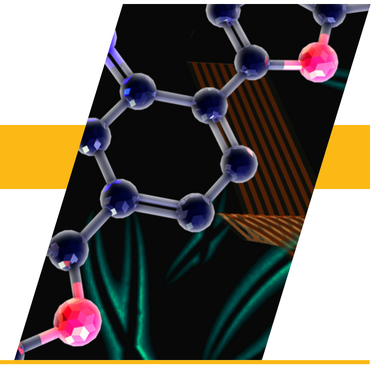
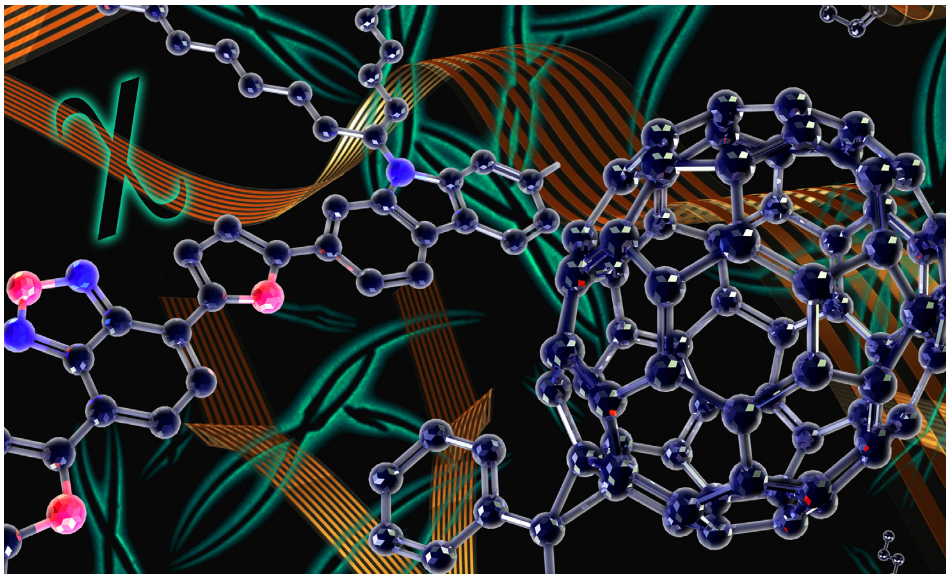


Rational Optimization of Organic Solar-Cell Materials



Artistic interpretation of an organic solar-cell mixture containing a blend of polymers and fullerenes. Interactions between these molecules (represented by the interaction parameter, χ) affect the degree of mixing that occurs in the photoactive layer, which in turn is key to device performance.

Scientific Achievement

Researchers have established a new quantitative model that connects molecular interactions in organic solar-cell materials to device performance.

Significance and Impact

The work suggests a way to quickly identify ideal material mixtures and processing methods, bypassing trial-and-error strategies and minimizing labor-intensive synthesis.

Improving efficiency–efficiently

To generate electricity from light, the photoactive layer of an organic solar cell (OSC) must allow the photoexcitation and separation of charges, something that can happen in blends of electron-donating and electron-accepting organic materials. Not surprisingly, such blends have been created in steady succession with the goal of improving device efficiency.

However, there are over a thousand combinations of electron donors and acceptors available for use in OSCs and countless processing variations. The reliance on trial and error to identify the best materials and methods is a serious limitation. A way to predict device efficiency based on easily measurable or derivable parameters would go a long way toward streamlining the process.

Flory–Huggins interaction parameter

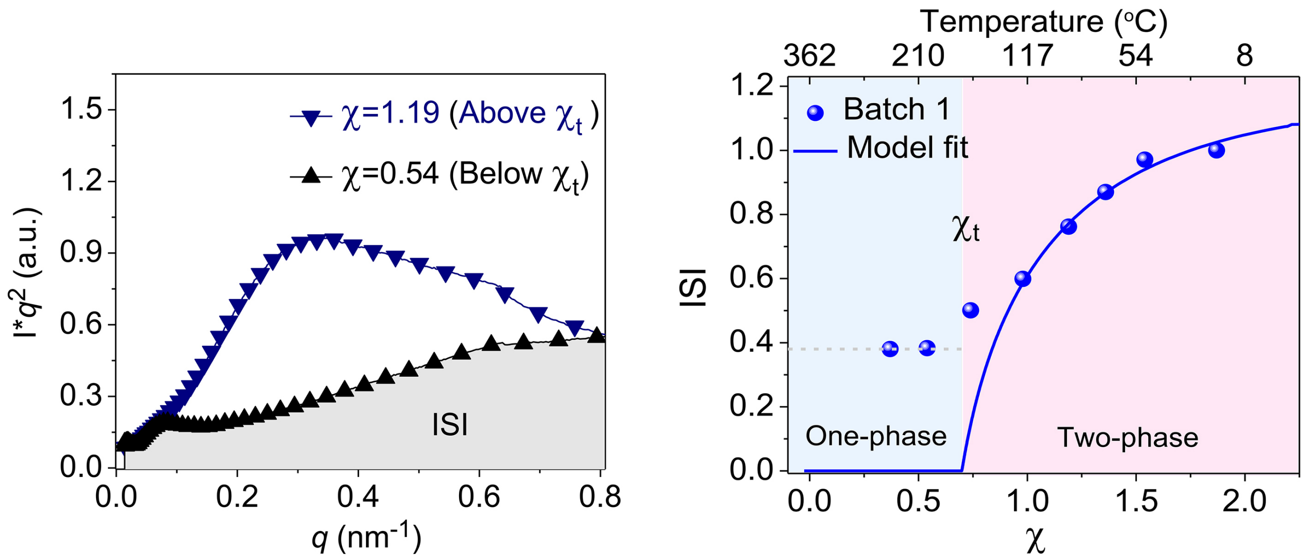
In this work, researchers studied a model OSC system consisting of a polymer (PCDTBT) and a fullerene ($PC_{71}BM$), the electron donor and acceptor, respectively. When added together, the materials may be phase-separated at a certain temperature and thus form two phases: a nearly pure fullerene-rich phase and a polymer-rich mixed phase. Because some mixing has to occur in order to separate charges, it's the polymer-rich mixed phase that largely controls device efficiency.

Using secondary-ion mass spectrometry (SIMS) at North Carolina State University, the researchers measured the polymer volume fraction in the mixed phase as a function of temperature. Based on this data, they determined the temperature-dependent Flory–Huggins interaction parameter χ for the system. This parameter measures the energy savings from mixing (or demixing) due to forces of attraction (or repulsion) between the molecules.

One-stop x-ray shop

At the ALS, three x-ray techniques were used for this work: resonant soft x-ray scattering (RSoXS) at Beamline 11.0.1, scanning transmission x-ray microscopy (STXM) at Beamline 5.3.2.2, and grazing-incidence wide-angle x-ray scattering (GIWAXS) at Beamline 7.3.3. The availability of both hard and soft x-ray probes at the ALS is invaluable in a project such as this, saving researchers time, energy, and money.

RSoXS is a unique tool for the determination of polymer structure with improved chemical sensitivity. The technique was used to measure the integrated scattering



Left: RSoXS scattering intensity vs angle for PCDTBT:PC$_{71}$BM films in the two-phase region (χ = 1.19) and the one-phase region (χ = 0.54); χ_t is the threshold value of χ between the phases. The area under each curve gives the integrated scattering intensity (ISI) for the corresponding value of χ. Right: Plot of several ISI values (from RSoXS measurements) against χ. In the one-phase region, where there is no phase separation, ISI remains constant. A sharp increase occurs as the phase separation sets in above the threshold χ_t (~0.72), and a subsequent leveling off is observed as the blend reaches saturation. This characteristic "constant-kink-saturation" shape observed also seen in measures of device performance.

intensity (ISI), a quantity related to domain purity. STXM provided quantitative information about the weight fraction of fullerene in the polymer matrix, and GIWAXS was used to characterize the molecular ordering in a variety of donor and acceptor materials, extending the work beyond the model system.

"Constant-kink-saturation" relation

The results establish a quantitative "constant-kink-saturation" relation between χ and ISI (a measure of domain purity) and between χ and a measure of device performance known as the fill factor. This relation holds across numerous high- and low-performing material systems, including fullerene and nonfullerene acceptors. Overall, the data reveal that a high fill factor (and thus better device performance) is obtained only when χ is large enough to lead to strong phase separation, with high purity of the mixed domains.

This work outlines a basis for using various experimental tests and future simulation methods to significantly reduce or eliminate trial-and-error approaches to material synthesis and device fabrication, maximizing efficiency for a given material system before laborious device optimization and complex syntheses are attempted.

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