Estimating χ in Blends for Organic Photovoltaic Devices

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Organic electrics based on π -conjugated polymers and small molecules are of broad commercial interest, offering a flexible, low-cost option for electronic devices. New organic photovoltaic (OPV) materials are developed at a rapid pace and require a robust set of analyses to quickly interrogate processability, morphology, and performance in functional solar cells. Most successful OPV devices are based on the bulk heterojunction (BHJ) structure, a morphology characterized by nanoscale separation of donor- and acceptor-rich domains. Separation is driven by thermodynamics, but is ultimately limited by kinetics during processing. Using differential scanning calorimetry (DSC), it is possible to selectively characterize the thermodynamics of phase separation. By probing the melting point depression of crystalline transitions in OPV blends, we can estimate the Flory-Huggins interaction parameter χ , which is a direct indicator of the segregation strength. The method is applicable to most OPV blended systems which typically contain a crystallizable, fullerene acceptor material. We also find internal consistency in estimations of χ using binary systems for which both the donor and acceptor materials are crystallizable. These systems provide two instances of melting point depression to by which to estimate and compare χ . DSC measurements are paired with grazing-incidence X-ray scattering results to correlate the segregation strength with the BHJ domain size.