Understanding the molecular weight dependence of photophysics, charge transport, morphology, and performance of all-polymer solar cells

Duyen Tran[1], Amélie Robitaille[2], Xiaomei Ding[1], Mario Leclerc[2], and Samson Jenekhe[1]

1. University of Washington, Seattle, Washington, United States
2. Universite Laval, Quebec, Quebec, Canada

All-polymer solar cells (all-PSCs) is a promising next-generation photovoltaic technology due to its unique advantages, including good mechanical flexibility, excellent thermal/mechanical durability, high visible transparency, and great potential for large-scale manufacture with low production cost. I will present our study of the effects of polymer number-average molecular weight (M_n) on the performance of all-PSCs. We used a series of biselenophene-napthalene diimide (PNDIBS) acceptor polymers synthesized by direct heteroarylation polymerization method with six M_n values spanning 20 – 130kDa and the donor polymer PBDB-T. We found that the short-circuit current and the power conversion efficiency (PCE) of all-PSC composed of PNDIBS/PBDB-T binary blends were maximized as M_n approached a critical value (M_n = 55kDa) but subsequently declined with further increase beyond the critical value. The blend photophysics, blend charge transport properties, and blend morphology were concurrently optimized at the critical M_n value. The underlying mechanism for the observed trends was explained by the efficient charge photogeneration rate, suppressed space-charge formation, superior and symmetric charge transport, and a bi-continuous network of ordered crystalline domains with predominant *face-on* molecular orientations at the optimal M_n. Our findings provide important structure-property relationship insights while providing design guidelines that are broadly applicable to the development of high-performance semiconducting polymers with optimal properties and enhanced photovoltaic properties.