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Entanglements in Conjugated Polymers[1] RENXUAN XIE, YOUNG-MIN LEE, MELISSA APLAN, NICK CAGGIANO, ENRIQUE GOMEZ, RALPH COLBY, Pennsylvania State Univ — Conjugated polymers, such as poly(3-hexylthiophene-2,5-diyl) (P3HT) and poly-((9,9-dioctylfluorene)-2,7-diyl-alt-[4,7-bis(thiophen-5-yl)-2,1,3-benzothiadiazole]-2',2"-diyl) (PFTBT), are widely used as hole and electron transport materials in a variety of electronic devices. However, fundamental knowledge regarding chain entanglements and nematic-to-isotropic transition is still lacking and are crucial to maximize charge transport properties. A systematic melt rheology study on P3HT with various molecular weights and regio regularities was performed. We find that the entanglement molecular weight Me is 5.0 kg/mol for regiorandom P3HT, but the apparent Me for regioregular P3HT is significantly higher. The difference is postulated to arise from the presence of a nematic phase only in regioregular P3HT. Analogously, PFTBT shows a clear rheological signature of the nematic-to-isotropic transition as a reversible sharp transition at 278 C. Shearing of this nematic phase leads to anisotropic crystalline order in PFTBT. We postulate that aligning the microstructure will impact charge transport and thereby advance the field of conducting polymers.

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Renxuan Xie
Pennsylvania State Univ

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