Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Regio regularity effects on chain mobility and entanglement for poly(3-hexylthiophene)[1] RENXUAN XIE, ENRIQUE GOMEZ, Department of Chemical Engineering, Penn State University at University Park, RALPH COLBY, Department of Materials Science and Engineering, Penn State University at University Park — Poly(3-hexylthiophene-2,5-diyl) (P3HT) is a conjugated polymer that can serve as the active layer in a variety of electronic devices. However, its glass transition temperature (T_α) and entanglement molecular weight (M_e) are still in dispute. These parameters are essential for estimating the density of tie chains, which are hypothesized to limit the bulk charge transport. A wide range of molecular weights of both regiorandom (RRa) and regioregular (RRe) P3HT were studied by oscillatory shear rheology. Coupled with the molecular weight distribution from GPC, M_e was extracted by fitting the linear viscoelastic data of multiple MW samples using BoB software. Furthermore, two T_αs were identified for both RRe and RRa P3HT. T_α corresponds to the segmental motion and follows Flory-Fox equation well for various MWs with 2 C $<T_\alpha<$14 C, yielding high MW limit of $T_{\alpha\infty}=21$ C. RRe has a larger M_e than RRa, which might originate from their different $T_{\alpha PE}$ corresponding to the side chain packing. So, further investigation on their packing lengths via dilute solution light scattering will be crucial to understand entanglement in these semiflexible polymers.

[1] National Science Foundation

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Date submitted: 06 Nov 2015

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