Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Poly-(3-hexylthiophene) Aggregate Formation in Binary Solvent Mixtures: An Excitonic Coupling Analysis DAVID BOUCHER, CALYNN JOHNSON, College of Charleston — We have studied the aggregation behavior of P3HT [$M_n \approx 28.2$ kDa, regioregularity >96 %, PDI ≈ 1.3] in 96 solvent mixtures is studied using UV-Vis absorption spectroscopy. We used Hansen solubility parameters (HSPs) and Spano excitonic coupling analyses to identify correlations between the properties of the solvent mixtures and the extent of structural order of the aggregates. It is clear that the identity of the poor solvent used to drive aggregation has a significant impact on the excitonic coupling behavior and, hence, the structural order of the P3HT aggregates. However, solubility parameter theory does not account nor provide a predictive theory for the observed trends. Instead, qualitative arguments based on the nature of the interactions between the solvents and the polythiophene and hexyl side chain motifs are used to rationalize the kinetics of formation and the observed excitonic coupling characteristics of the P3HT aggregates.

David Boucher
College of Charleston

Date submitted: 06 Nov 2013 Electronic form version 1.4