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Estimating the Magnitude of Exciton Delocalization in Regioregular P3HT through Computational Modeling and Transient Absorption Spectroscopy MICHAEL HEIBER, ALI DHINOJWALA, The University of Akron — Exciton delocalization has been shown to have a potentially strong impact on the performance of organic solar cells. However, very few attempts have been made to estimate the magnitude of exciton delocalization in common semiconducting polymers. We show how the magnitude of exciton delocalization can be extracted from two types of femtosecond transient absorption spectroscopy experiments using computational modeling tools. By fitting exciton delocalization models to previously published experimental data, we extract two separate estimates of the magnitude of exciton delocalization in regioregular poly(3-hexylthiophene) (P3HT). First, fitting exciton-exciton annihilation behavior in pristine P3HT films leads to an estimation of the exciton delocalization radius of 1.6±0.25 nm. Second, dynamic Monte Carlo modeling of the exciton dissociation dynamics for a P3HT:PCBM blend film results in a second approximation of the exciton delocalization radius of 1.9±0.6 nm. These estimates are significantly smaller than previously published values and provide strong evidence for less delocalization than used in previous device models.

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