

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Chromophoric disorder in conjugated polymers: the curious case of P3HT LENA SIMINE, Rice University, PETER ROSSKY, Dept. of Chemistry, Rice University — The origin of the broad absorption spectrum of conjugated polymers is discussed. Motivated by the open questions posed in the recent experimental literature, we investigate theoretically the chromophoric disorder in single molecule poly(3hexyl)thiophene (P3HT) at the atomic level using quantumclassical simulations. We reproduce the absorption spectrum and confirm qualitatively the prediction of simplified models the localization length of the first excited state decreases with increasing temperature. Counter to expectation, the same trend is observed for the the average energy of the chromophore: in spite of a shorter localization length, the spectrum of the hot chromophore is redshifted with respect to its cold counterpart. We trace this peculiarity to the anharmonicity of the underlying torsional potential which allows preferential access to more planar interring conformations at high temperature. The contributions of bending to the transitional energies, the origin of inhomogeneous broadening and the possibility of classification of the chromophore as planar/twisted/bent at low and high temperatures are discussed.

Lena Simine
Rice University

Date submitted: 15 Dec 2015

Electronic form version 1.4