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Neutron Vibrational Spectroscopy and modeling of polymer/dopant interactions ADAM MOULE, THOMAS HARRELSON, University of California, Davis, YONGQIANG CHENG, ANIBAL RAMIREZ-CUESTA, Oak Ridge National Lab, ROLAND FALLER, University of California, Davis, DAVID HUANG, University of Adelaide, Australia — Neutron vibrational spectroscopy (VISION and ORNL) is a powerful technique to determine the configurations of organic species in amorphous samples. We apply this technique to samples of the semiconducting polymer regio-regular P3HT to determine the molecular configurations outside of the crystalline domains, which have never been investigated. Application of density functional theory modeling using crystal field theory and for the single molecule approach yield a variety of configurations of the polymer backbone and side chains. These results demonstrate that only 1% of the volume corresponds to the assumed crystal structure solved using x-ray diffraction. In addition we investigate the configurations of P3HT doped with the molecular dopant F4TCNQ and determine that the charging of the polymer backbone leads to increased side chain stiffness. These results have significant implications for design of organic electronic devices based on thiophenes.

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