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An Improved Forcefield for Molecular Modeling Oof Crystalline Poly(3-Hexyl Thiophene)[1] RAM BHATTA, Department of Chemistry, University of Akron, YENENEH YIMER, Department of Polymer Science, University of Akron, DAVID PERRY, Department of Chemistry, University of Akron, MESFIN TSIGE, Department of Polymer Science, University of Akron — A fundamental understanding of molecular structure and dynamics of poly(3-hexyl thiophene) (P3HT), one of the most promising organic solar cell materials, is crucial for improving the efficiency of organic solar cells containing P3HT as the donor. Molecular dynamics (MD) simulations can produce the correct structures and dynamics of P3HT provided that robust forcefields are employed for this system. The forcefields that are currently used for MD simulations of P3HT are mostly taken from the analogous thiophene molecule, bi-thiophene. However, such forcefields may lack to produce the correct morphology and stacking properties of P3HT. We present the results of MD simulations using an improved forcefield for P3HT. In the improved forcefield the torsional and partial atomic charge parameters for both the alkyl side chains and backbone were derived from ab initio calculations. Our results from MD simulations are compared with available experimental and theoretical data and the range of accessible structures is explored.

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