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Modeling chain configurations of conjugated polymers as a function of charge concentration[1] BRANDON WOOD, Univ of California - Berkeley, YONGWOO SHIN, Lawrence Berkeley National Laboratory, KRISTIN PERSSON, Univ of California - Berkeley — Conjugated polymers are promising materials for energy storage and energy conversion applications due to their electronic and optical properties. The electronic structure of conjugated polymers plays an important role in determining individual chain configurations due to electron-phonon coupling interactions. In this work, we evaluated chain properties and configurations as a function of charge concentration using a simplified model based on first-principles calculations that captures the electronic structure changes. Our computations indicate that the charge concentration modifies the backbone stiffness in polythiophenes, which is manifested by changes in classical properties such as persistence length and end-to-end distance.

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