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Electric Field and Electron-Electron Interactions Effects on Bipolaron Transport in Polythiophene[1] YAPING LI, JOLANTA LAGOWSKI, Memorial University of Newfoundland — Polythiophene is one of the most widely used organic conjugated polymer. Its charge transport mechanism has been a subject of many intensive studies. We employ the extended Su-Schriefer-Heeger's theoretical model (SSH), including electric field and electron-electron interactions, to study bipolaron transport in polythiophene. This model involves the solution of coupled equations, consisting of the time-dependent Schrodinger equation and the classical motion equation for the lattice displacement, which are solved numerically in a self-consistent way. The time-dependent unrestricted Hartree–Fock approximation is also used. The parameters employed in the computations are determined by requiring good agreement with theoretical and experiment values for band gap and bond lengths. We find that a bipolaron does not distort in a weak electric field, however, a strong electric field can dissolve it, transforming localized charges into free charges. Electron- electron interactions do not significantly affect the nature of bipolaron transport in polythiophene.

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