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The complex band perspective of self-localization in conducting polymers QING LU, MINGHAI LI, LAUREN O'MALLEY, XI LIN — The complex band is an extension of the conventional band structure to allow Bloch wavevector being a complex number, so that energy becomes a continuous function of the complex wavevector. Imaginary wavevectors mark the characteristic wavefunction decay rate for those states existing in the forbidden gaps, and thus provide the localization perspective of these defect states. This view, however, has been rarely discussed concerning of self-localized solitons and polarons in conducting polymers. In this work, we use the Su-Schrieffer-Heeger (SSH) model and its extended model to compute the complex band structures of the defect-free *trans*-polyacetylene (t-PA) and poly-(p-phenylene-vinylene) (PPV) chains, respectively. We find the complex wavevectors predicted by the complex band structure computations agree excellently with the decay rates of the soliton wavefunction in t-PA and the bipolaron wavefunction in PPV. From this complex band perspective, our recently revealed multiple self-localized electronic states induced by either the electron correlation or the Peierls twin instability can be easily understood.

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