Abstract Submitted
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An adapted Su-Schrieffer-Heeger Hamiltonian for conducting polymers MINGHAI LI, XI LIN, Boston University, Mechainical Engineering Dept — We present an adapted Su-Schrieffer-Heeger (SSH) model Hamiltonian to naturally incorporate the materials-specific properties of various conducting polymers, such as poly-(p-phenylene-vinylene) (PPV), polypyrrole (PPy), polyaniline (PANI), and their functional derivatives. Taking PPy as an illustrating example, we treat heterogeneous NH sites in pyrrole as positive ions, or attractive potential wells for π electrons. All parameter values are determined by numeric fitting to *ab-initio* calculations and experimental data. The model has excellent agreements with *ab-initio* calculations and experimental data in both the equilibrium configurations and π electron structures for the cases of a pyrrole ring, a pyrrole dimer, and a long chain of 20 pyrrole rings. Polarons and bipolarons were found upon charge dopings. Results on the porphyrin model Hamiltonian are discussed.

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