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New conduction mechanism in doped trans-polyacetylene through soliton-bipolaron transition ANDRE BOTELHO, MINGHAI LI, XI LIN, Boston University — By considering the independent movement of a soliton and an anti-soliton in a periodic boundary condition, a new mechanism arises for soliton motion. First, the soliton (anti-soliton) moves while the anti-soliton (soliton) remains pinned by the ion. The soliton and anti-soliton then form a locally stable bipolaron. From this local minimum, the bipolaron can dissociate into its original soliton/anti-soliton pair, with one remaining pinned and the other moving towards an empty ion site. This mechanism has lower energy than when considering the motion of a single soliton in a periodic boundary condition. Energies were calculated using an SSH model with an added Coulombic interaction between each CH site and positive ions in a regular lattice. The model was treated in the Hartree Fock approximation and transition points calculated through the nudged elastic band (NEB) method.

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