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Adapted Su-Schrieffer-Heeger Hamiltonian for PPV, PPP, and polyacenes YONGWOO SHIN, XI LIN, Boston university — This work presents a unified model Hamiltonian for poly-*p*-phenylenevinylene (PPV), poly-*p*-phenylene (PPP), and polyacenes based on the classical Su- Schrieffer-Heeger Hamiltonian for polyacetylene, with one single extra electron- phonon coupling parameter. Predicted band gaps of all these polymers and their oligomers of all lengths closely match to the available experimental results, with an accuracy exceeding the time-dependent density functional theory. Self-localized polaron states and their mobility are computed without any constraints.

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