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A unified model Hamiltonian for polythiophene, polypyrrole, polyfuran, free base porphyrin, and polyaniline: Accuracy, transferability, and computational efficiency ANDRE BOTELHO, XI LIN, Division of Materials Science and Engineering, Boston University, Boston MA — Two fully transferable physical parameters are incorporated into the historical Su-Schrieffer-Heeger Hamiltonian to model conducting polymers beyond polyacetylene, one parameter γ scales the electron-phonon coupling strength in aromatic rings and the other parameter ε specifies the heterogeneous core charges. This generic Hamiltonian predicts the fundamental band gaps of polythiophene, polypyrrole, polyfuran, free base porphyrin, polyaniline, and their oligomers of all lengths with an accuracy exceeding the time-dependent density functional theory. Additionally, its computational costs are four orders of magnitude or more lower than first-principles approaches.

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