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Model Hamiltonian for predicting the bandgap of conjugated systems ANDRE LEITAO BOTELHO, YONGWOO SHIN, XI LIN, Division of Materials Science and Engineering, Boston University — We calculate the bandgaps for conjugated systems using the adapted Su-Schrieffer-Heeger Hamiltonian and find good agreement with 130 independent experimental points. The 2D version of the model correctly demonstrates the decrease in bandgap from the addition of vinylene bridges to both poly(*p*-phenylene) and polythiophene indicating that planarization is not a significant effect. Expanding the model to 3D shows that interchain interactions systematically reduces the bandgap. In fused rings sharing dissimilar bonds, such as in isothianaphthene, the bond length dimerization along the carbon backbone decreases leading to a decrease in the bandgap. In contrast, when fusing two of the same rings along equivalent bonds, for example thienoacene, the bandgap change is less than 10% at best when normalized by the number of carbon atoms in the conjugation path. From porphyrin and pyrrole-benzothiadiazole we learn that tautomerization significantly affects the bandgap, as the ε value for NH had to be used for both NH and N, indicating that H is being shared by both. In modeling donor-acceptor co-polymers we accurately calculate the reduction in the bandgaps when compared to their parent homopolymers.

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