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Computational materials design for bulk heterojunction solar cells XI LIN, YONGWOO SHIN, Boston University — The adapted Su-Schrieffer-Heeger Hamiltonian is further developed in this work to predict the optical bandgaps of more than 200 different π-conjugated systems. Insights on the structure-property relationship of these π-conjugated systems lead to guiding rules for new photovoltaic materials design. A copolymer of parallel and perpendicular benzodithiophenes, differing only in sulfur atom locations, is proposed as a candidate to achieve the optimal 1.2 eV donor optical gap for organic photovoltaics. The charge transfer mechanisms and the exciton and charge carrier mobilities are computed and compared for various bulk-heterojunction structures to improve the overall power convention efficiency.

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