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Computational design of co-polymer electron donors for bulk heterojunction photovoltaic solar cells YONGWOO SHIN, JIAKAI LIU, XI LIN, Boston University — In this work, our recently developed adapted Su-Schrieffer-Heeger Hamiltonian is used to systematically explore the optoelectronic properties of thousands of pi-conjugated structures. New physical insights on the structure-property relationship are extracted and transformed into practical guiding rules in the donor materials design. For the power-efficient copolymer structures, we find that the energy variation of frontier orbitals can be controlled either independently or collectively, depending on their specific donor or acceptor structures. In particular, we find that having five-membered conjugated carbon rings in the acceptor units is essential to break the electron-hole charge conjugation symmetry, so that the LUMO levels of the copolymer can be reduced dramatically while holding the HOMO energy levels in the donor units constant. On the other hand, by incorporating heteroatoms into the donors units, we can vary the HOMO levels of the copolymers independently. Effects of introducing various side groups (-R, -O, -CO, -COO, and thiophene) on the primitive donor and acceptor structures are investigated and their results are discussed in details. Finally, unexpected localized states are found, for the first time, in our calculations for a few special co-polymer structures. These localized states, with electrons localized on one end of the copolymer chain and holes on the other end, contain large dipole moments and therefore may be treated as a new design dimension when these copolymers are placed in polar and non-polar solvent environments.

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