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Halogenated contorted hexabenzocoronenes as electron acceptors in organic solar cells ANNA HISZPANSKI, LEO SHAW, Chemical and Biological Engineering, Princeton University, MATTHEW BRUZEK, Chemistry, University of Kentucky, Lexington, JONATHAN SAATHOFF, Chemical Engineering, Cornell University, LAURA KRAYA, FRANSIZKA LEUTTICH, Electrical Engineering, Princeton University, MICHAEL BRADY, MICHAEL CHABINYC, Materials Science, University of California, Santa Barbara, ANTOINE KAHN, Electrical Engineering, Princeton University, PAULETTE CLANCY, Chemical Engineering, Cornell University, JOHN ANTHONY, Chemistry, University of Kentucky, Lexington, YUEH-LIN LOO, Chemical and Biological Engineering, Princeton University
— Substituting hydrogens with fluorines and chlorines lowers the lowest unoccupied molecular orbital (LUMO) of organic semiconductors, thereby facilitating electron injection into and electron transport in these materials. We synthesized contorted hexabenzocoronene (HBC) derivatives with increasing fluorine- and chlorine-substitution. While the LUMO of fluorinated HBCs decreases by 60 meV/F, the LUMO of chlorinated HBCs decreases by 70 meV/Cl, resulting in slightly narrower bandgaps in the chlorinated compounds. Interestingly, only the chlorinated HBCs are electrically active. Bulk-heterojunction solar cells with poly(3-hexyl thiophene) as the polymer donor have yielded efficiencies as high as 1.1%. We believe the drastic difference in electrical activity between the two nominally similar families of HBCs to stem from differences in their solid-state packing. This observation underscores the importance of structure-property relationships in guiding electron acceptor design.

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