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Halogenated contorted hexabenzocoronene derivatives for electron transport in thin-film transistors and organic photovoltaics ANNA HISZPANSKI, LEO SHAW, Chemical and Biological Engineering Dept., Princeton University, MATTHEW BRUZEK, Chemistry Dept., University of Kentucky, FRANZISKA LUETTICH, ANTOINE KAHN, Electrical Engineering Dept., Princeton University, JOHN ANTHONY, Chemistry Dept., University of Kentucky, YUEH-LIN LOO, Chemical and Biological Engineering Dept., Princeton University
— In investigating electron acceptor substitutes for fullerene derivatives in organic photovoltaic applications, we have modified a semiconductor, contorted hexabenzocoronene (HBC), with halogens to increase its oxidative stability and lower its lower unoccupied molecular orbital energy level relative to vacuum level. We synthesized a series of HBC derivatives with increasing fluorine substitution on the peripheral aromatic rings and elucidated the effect of chemical modification on electronic properties. Though we observe a 57 meV shift in both the highest occupied and lowest unoccupied energy levels of the molecules with each progressive addition of fluorine, none of the fluorinated HBC derivatives demonstrate electron transport in thin-film transistors. By substituting chlorine for four of the peripheral fluorines, however, this mixed-halogenated compound exhibits n-transport characteristics. Unoptimized thin-film transistors comprising 8F-8Cl-HBC have demonstrated electron mobilities as high as 0.01 cm^2/Vs, and unoptimized bulk-heterojunction solar cells with poly(3-hexyl thiophene) as the polymer donor have yielded power conversion efficiencies as high as 0.9%.

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