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Heteroatom-Containing Contorted Molecular Semiconductors
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— Contorted polyaromatic hydrocarbons (c-PAHs), such as contorted hexabenzocoronene (c-HBC), are promising active ingredients for organic photovoltaic (OPV) devices due to their inherent stability, tunable frontier energy levels, and synthetic accessibility. The utility of c-HBC derivatives in OPV devices, however, has been limited by the large band gaps of these materials and, as a consequence their limited ability to harvest visible light. Here we report the synthesis, characterization and device integration of tetrabenzofuranyldibenzocoronene (c-TBFDBC) and tetrabenzothienodibenzocoronene (c-TBTDBC) – a pair of heteroatom-containing c-PAHs that show broader absorption of the solar spectrum compared to c-HBC, with maximum absorptivities above 10^5 M^{-1} cm^{-1} in both the near-UV and in the visible. Bilayer OPV devices comprising c-TBFDBC or c-TBTDBC and C70 outperform those having c-HBC in photocurrent production and power conversion efficiency. External quantum efficiency spectra indicate improved light harvesting by both donor and acceptor molecules on annealing. Grazing incidence x-ray diffraction experiments reveal increases in the crystallinity of donor and acceptor layers on annealing and a preference for edge-on orientation in c-HBC and c-TBFDBC.

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