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Title: High Hole Mobility and Efficient Ambipolar Charge Transport in Heterocoronene-Based Ordered

Columnar Discotics

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Abstract:

Heterocoronene, a new redox-active core fragment, is utilized for the synthesis of room-temperature columnar discotic liquid crystals (DLCs). Three wedge-shaped side chains having different lengths of alkyl tails are introduced at the periphery of the heterocoronene core to prepare three kinds of discotic molecules, 1 (R = C10H21), 2 (R = C12H25), and 3 (R = C14H29). X-ray diffraction (XRD) analysis confirmed the packing variation in the columnar lattices regulated by alkyl chains of discrete length and steric bulk. When used in space charge limited current devices, compound 1 exhibits a high hole mobility value of 8.84 cm2/V s at ambient temperature, whereas compounds 2 and 3 show efficient ambipolar charge transport behavior with maximum hole (μ h) and electron (μ e) mobilities of 0.70 and 3.59 cm2/V s, respectively, for compound 3. The mobility values (μ h = 8.84 cm2/V s for 1 and μ e = 3.59 cm2/V s for 3) are remarkable and the highest ever disclosed for any DLC-based organic semiconductor, promising to deliver a good balance between mobility and processability in devices. The grazing incidence small- and wideangle X-ray scattering experiments are employed to quantify the extent of alignment in the film state, which correlates with the observed trend of mobility values.

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