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Electronic Supplementary Information

High-mobility, high-luminescence and low-threshold pentacene-doped cyano-substituted distyrylbenzene crystal

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The thickness of one layer is in good agreement with the dimension of the unit cell parameter *c* (15.611 Å), which indicates that the layer-by-layer growth in the crystal is along the *c* axis and the crystal surface corresponds to the *ab* plane of unit cell. Thus, the long axes of the 2-CSB molecules form an angle of 60° with respect to the crystal surface. On the basis of the crystal structure, we draw the molecular stacking mode in the molecular layer, as shown in Fig. S1. As can be seen, all of the molecules are packed in the same orientation along the *a* axis, in which intermolecular π overlap stacks will benefit for the carrier transport in the 2-CSB crystal-based field-effect transistors.

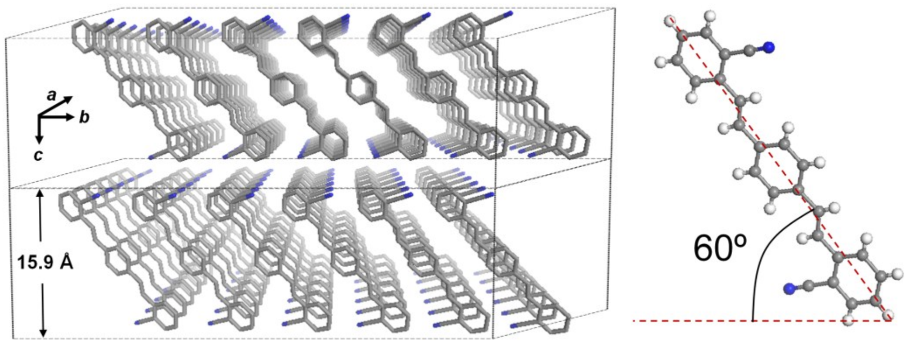

Fig. S1 Oriented alignment of the molecules in the crystal: the height of the molecular layer (15.9 Å) from AFM and XRD results corresponds to the length of 2-CSB molecule along the *c* axis direction vector; and the angle of the molecular long axis with *ab* plane is 60° shown in the right side.

The electronic absorption and emission spectra were calculated at TD-B3LYP functional and 6-311G(d,p) basis set.

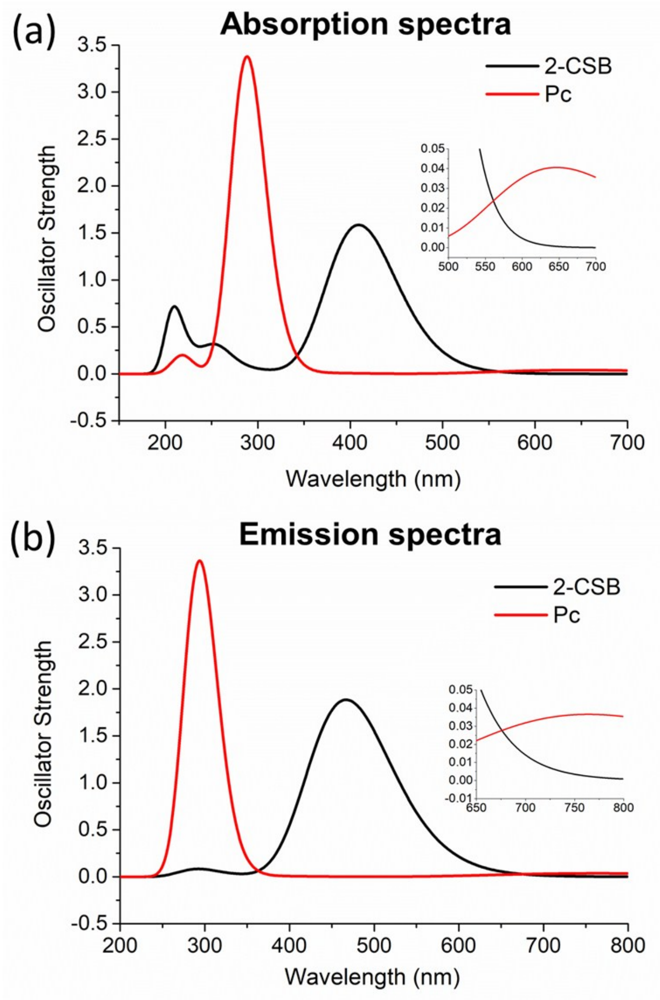

Fig. S2 The calculated absorption (a) and emission (b) spectra of 2-CSB molecule and Pc molecule. Insert figures are the drawings of partial enlargement at the long wavelength regions.

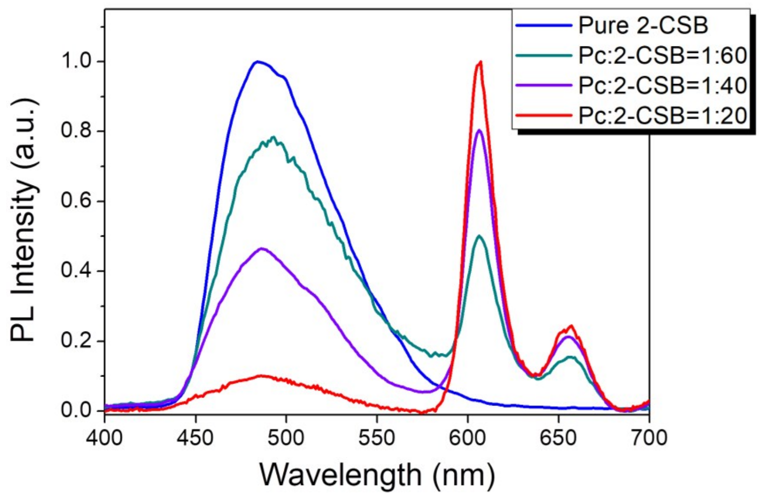

Fig. S3 The emission spectra of pure 2-CSB crystal and 2-CSB⊂Pc crystals with different weight ratios of Pc to 2-CSB (1:60, 1:40, 1:20).

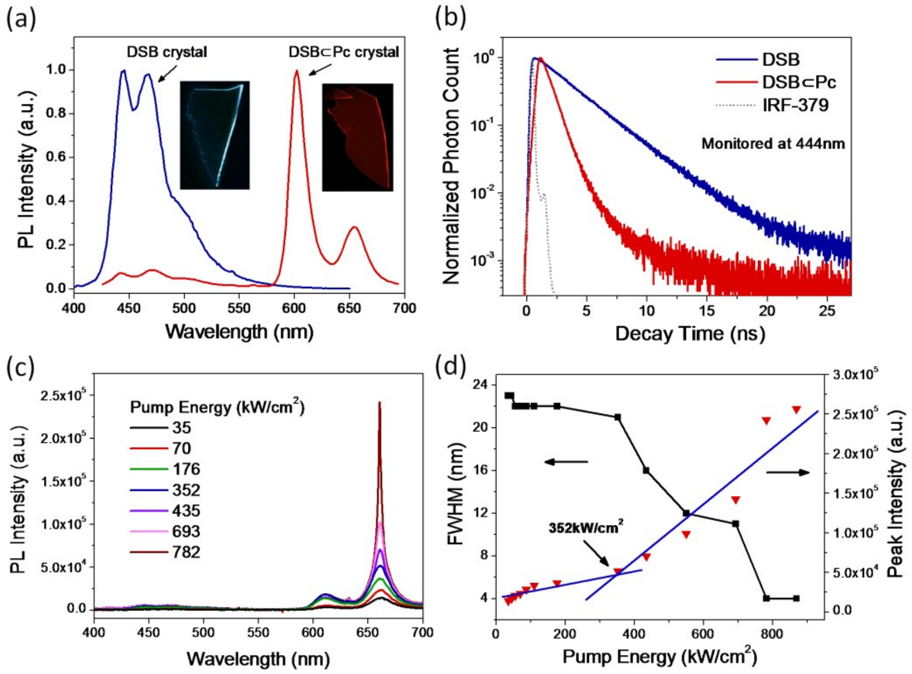

Fig. S4 (a) The emission spectra of DSB crystal and DSB⊂Pc crystal; and the absorption and emission spectra of the Pc solution in chloroform. Insert figures are the optical photographs of corresponding crystals under the ultraviolet lamp; (b) Time-resolved fluorescence decay curves of DSB crystal and DSB⊂Pc crystal monitored at the emission wavelength of 444 nm; (c) PL spectra of a slice-like DSB⊂Pc crystal as a function of the pump laser energy; (d) Dependence of the peak intensity and FWHM of the PL spectra on the pump laser energy.

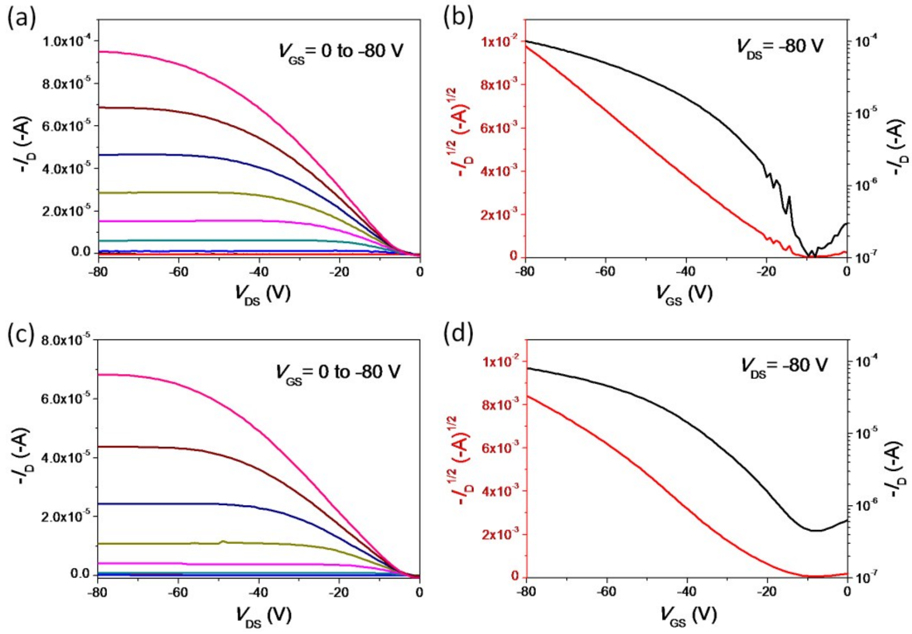

Fig. S5 (a, b) Output and transfer characteristics of 2-CSB crystal-based OFET, which give the mobility of 0.66 cm^2/Vs with channel length of 100 μm and width of 500 μm; (c, d) Output and transfer characteristics of 2-CSB⊂Pc crystal-based OFET, which give the mobility of 0.51 cm^2/Vs with channel length of 100 μm and width of 760 μm.

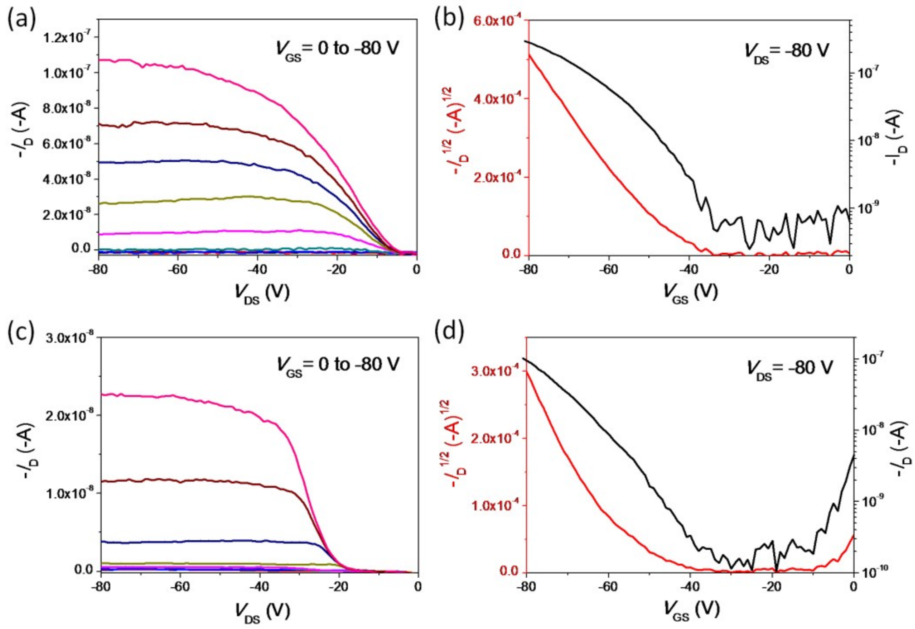

Fig. S6 (a, b) Output and transfer characteristics of DSB crystal-based OFET, which give the mobility of 7.5×10^{-3} cm^2/Vs with channel length of 100 μm and width of 650 μm; (c, d) Output and transfer characteristics of DSB⊂Pc crystal-based OFET, which give the mobility of 3.6×10^{-3} cm^2/Vs with channel length of 100 μm and width of 750 μm.