Controlled Transition Dipole Alignment of Energy Donor and Energy Acceptor Molecules in Doped Organic Crystals, and the Effect on Intermolecular Förster Energy Transfer

Huan Wang,[b] Bailing Yue,[b] Zengqi Xie,*[a] Bingrong Gao,[c] Yuanxiang Xu,[b] Linlin Liu,[a] Hongbo Sun[c] and Yuguang Ma*[a,b]

[a] State Key Laboratory of Luminescent Materials and Devices, Institute of Polymer Optoelectronic Materials and Devices, South China University of Technology, Guangzhou 510640, P. R. China. Fax: 86 20 87110606; Tel: 86 20 87114346; E-mail: ygma@scut.edu.cn, msxiez@scut.edu.cn

[b] State Key Laboratory of Supramolecular Structure and Materials, Jilin University, Changchun 130012, P. R. China

[c] State Key Laboratory on Integrated Optoelectronics, Jilin University, Changchun 130012, P. R. China

Table of Content:

1. Preparation of the doped crystals

The sublimated molecules transport with carrier gas (Ar, 99.999%), and the doped crystals grow in the crystal growth zone (relative low temperature zone). After two or three days of growth, large size slice crystals formed hanging inside of the growth tube. The doping concentrations in the doped crystals were tuned by changing the crystal growth conditions.

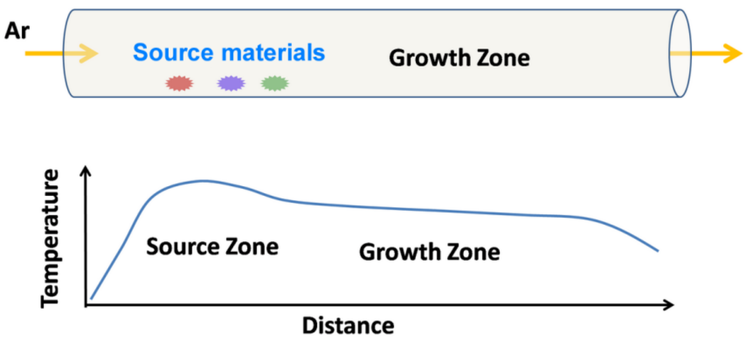

Figure S1. Schematics of the apparatus for the growth of doped crystals by physical vapor method. The temperature in the apparatus was controlled as shown in the bottom.

In order to verify the reproducibility of the preparation of the white light emitting doped crystal, the experiment was repeated for 3 times. The obtained crystals were subjected to PL measurement and the PL spectra are shown in Fig. S2. The CIE coordinates are summarized in Table S1 and shown in Fig. S2e.

Table S1. The conditions and CIE coordinates summaries of tetracene and pentacene -doped *trans*-DSB crystals with different color emission obtained by modulating the heated temperature of materials.

Conditions	Pentacene	*trans*-DSB	Tetracene	CIE coordinates (x, y)
(a)	250 ºC	210 ºC	150 ºC	(0.33, 0.39)
(b)	250 ºC	210 ºC	150 ºC	(0.36, 0.37)
(c)	250 ºC	210 ºC	150 ºC	(0.34, 0.33)
(d)	240 ºC	190 ºC	140 ºC	(0.24, 0.38)

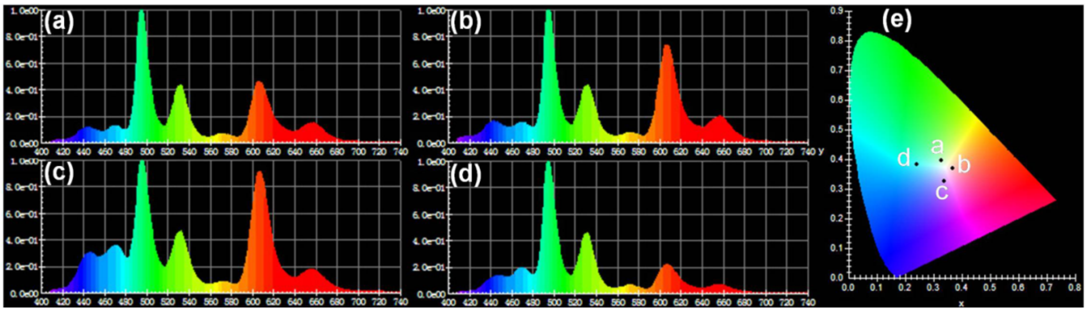

Figure S2. The PL spectra of tetracene and pentacene -doped *trans*-DSB crystals. The conditions for different samples are shown in Table S1.

2. Determination of the doping concentrations in the doped crystals

Chromatograph analysis was used to determine the guest-host mol ratios of Tc, Pc and DSB in the doped crystals prepared under different experimental conditions. One example is given as following. Firstly, a standard solution with mole ratios of Tc:DSB:Pc=1:10:1 was prepared and subjected to chromatograph analysis. As shown in Fig. S3a, there were three signals with different retention times of 13 min, 24 min and 29 min that correspond to Tc, DSB and Pc respectively. Then, the doped crystals were dissolved and analyzed by chromatograph under the same conditions. By comparing the integral areas of the signals for Tc, DSB and Pc of the samples with those of the standard, the mole ratios between the three components were determined, as shown in Fig. S3 b and c.

The same method was applied to determine the mole ratios of two components in DSB⊂Tc, DSB⊂Pc and Ac⊂Tc crystals.

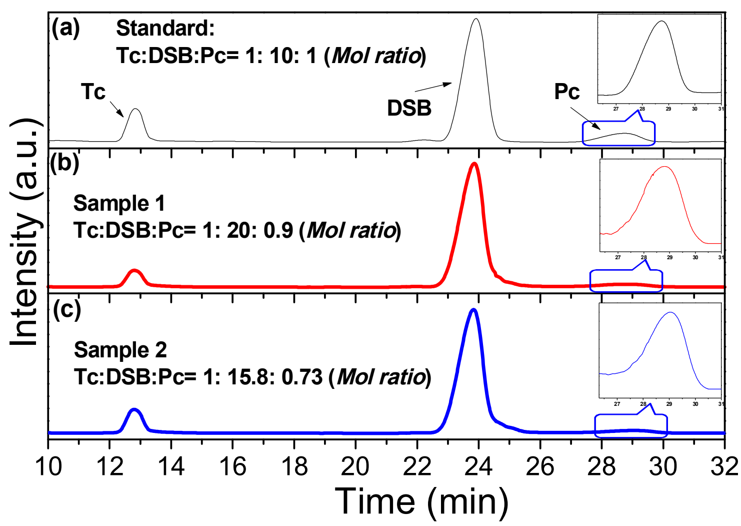

Figure S3. The chromatograph graphs of the mixture of Tc, DSB and Pc with different mol ratios. (a) Standard with Tc:DSB:Pc=1:10:1; (b, c) the mole ratios of the three components were determined to be Tc:DSB:Pc=1:20:0.9 and 1:15.8:0.73 respectively, by comparison with the standard.

3. Morphological and structural characterization

Fig. S4a shows the AFM height image at the edge areas of the DSB⊂Tc-Pc crystal (DSB: Tc: Pc= 20:1:0.9). Step-like morphology has been found. From the cross-section analyses, the average height of steps observed on the crystal surface is about 1.78 nm, which corresponds to the length of DSB molecule. Fig. S4b shows the diffraction patterns of XRD on the slice crystal. As can be seen, the diffraction peaks occur equidistantly with angle degree varying, and the diffraction peaks are very sharp, so the doped crystal have the good ordered layer-by-layer structures. According to the Bragg equation the thickness of one molecular layer of DSB⊂Tc-Pc crystal is calculated to be 1.76 nm, which corresponds to the one-step height of the doped crystal in AFM image.

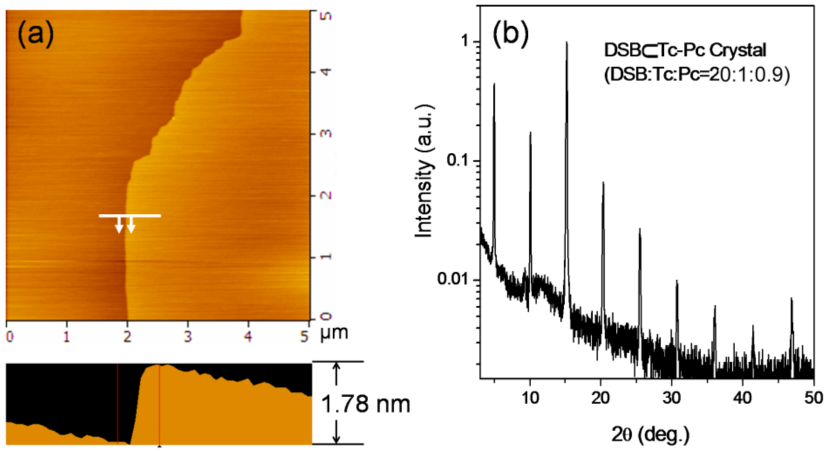

Figure S4. (a) AFM height image of the surface of DSB⊂Tc-Pc crystal (DSB: Tc: Pc= 20:1:0.9) and its enlarged sectional analysis. (b) Wide-angle X-ray diffraction patterns of DSB⊂Tc-Pc crystal (DSB: Tc: Pc= 20:1:0.9).

4. Preparation of Tc doped Ac film

Because Ac tends to form micro crystals during fabrication of the film by spin-coating method, we try to disperse both Ac and Tc by polystyrene (PS). The amount of Ac (by weight) was increased step-by-step, keeping Tc (1) and PS (1000) as constants. As shown in Figure S5, when the amount of Ac changed from 200 to 300, the energy transfer efficiency from Ac to Tc keep as ~85%. So we use the ratio of 1000:200:1 (PS:Ac:Tc) to calculate the distance between host and guest molecules.

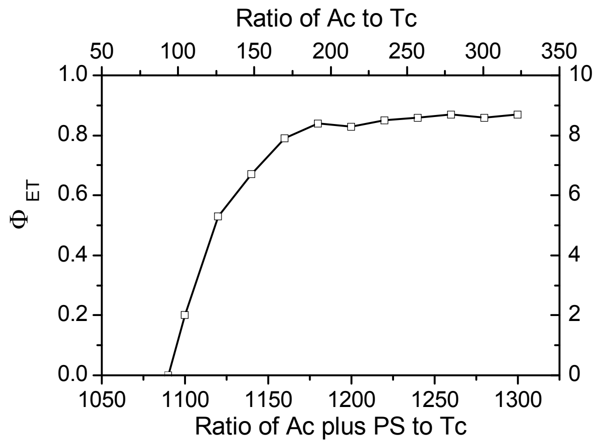

Figure S5. Energy transfer efficiency in doped films.