

## **Supplementary material:**

### **Effect of Configurational Isomerism and Polymorphism on Chalcone Fluorescent Properties**

Ruimin Zhang, † Mingliang Wang†\*, † Hao Sun, † Arshad Khan, † Rabia Usman, †

Shengzhi Wang, † Xiantao Gu, † Jia Wang and Chunxiang Xu ‡\*

*† School of Chemistry and Chemical Engineering, Southeast University, Nanjing 211189,*

*P. R. China*

*‡ State Key Laboratory of Bioelectronics, Southeast University, Nanjing 210096, P. R.*

*China*

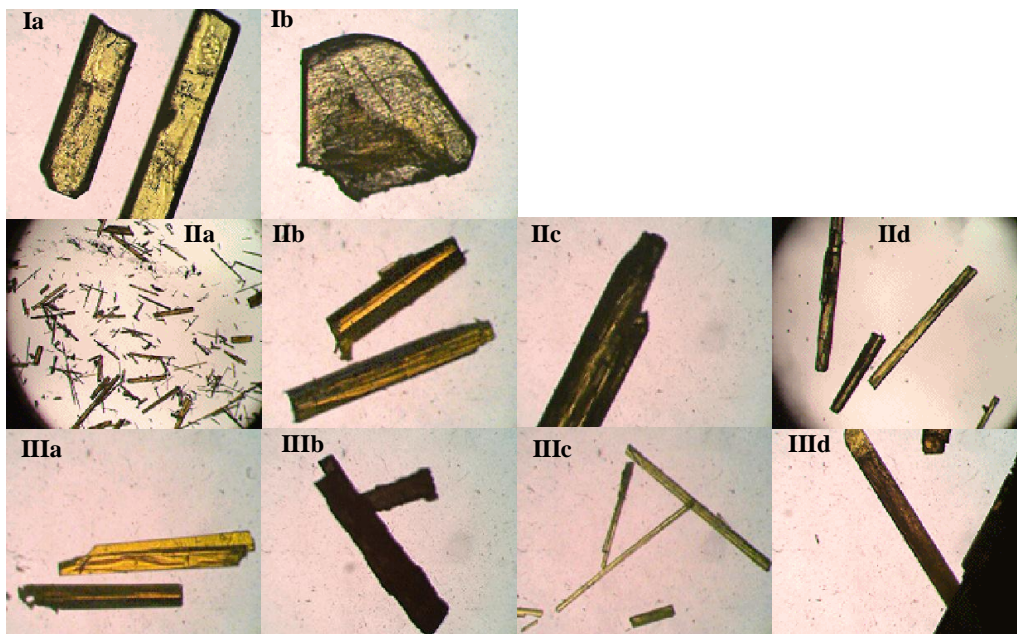


Figure S1. Microscopy graphs of all forms.

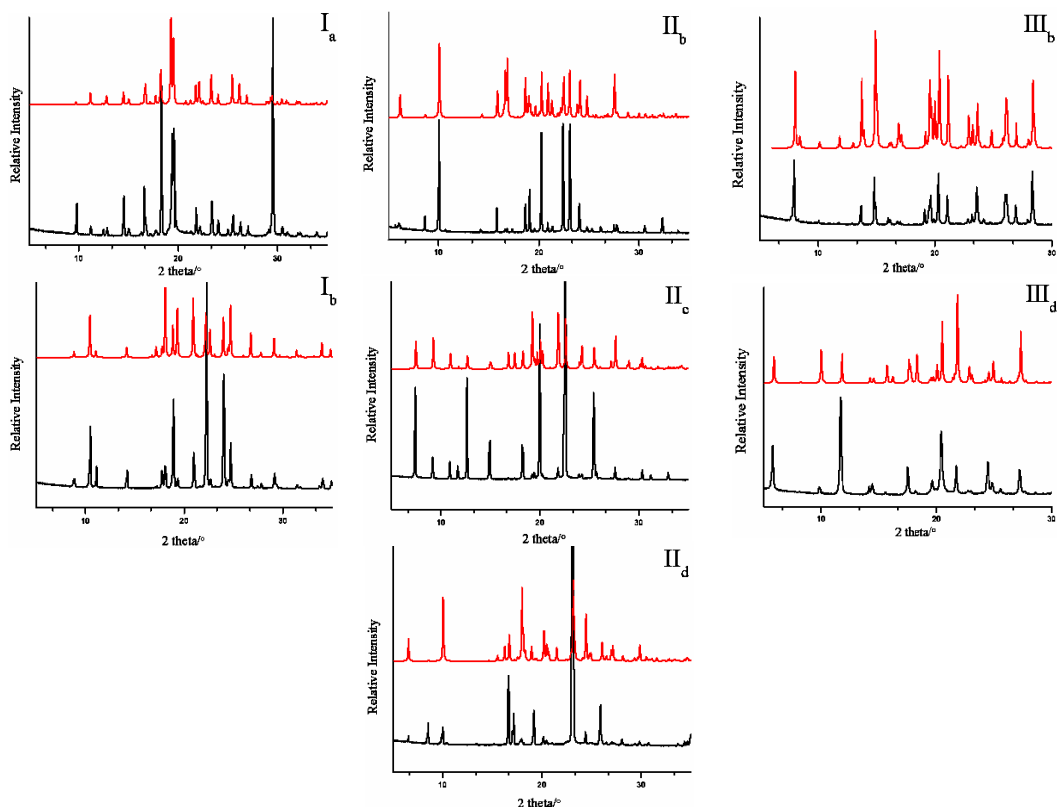
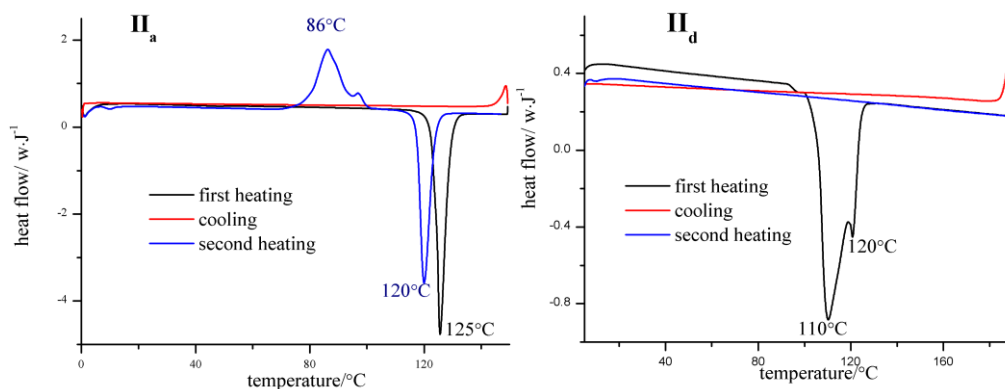
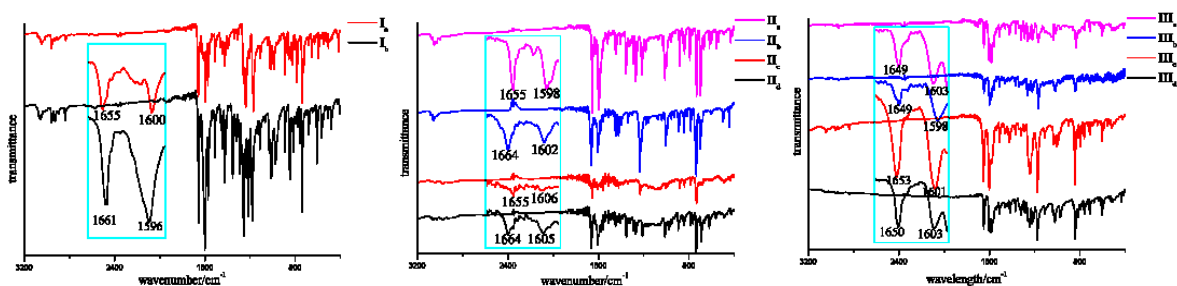


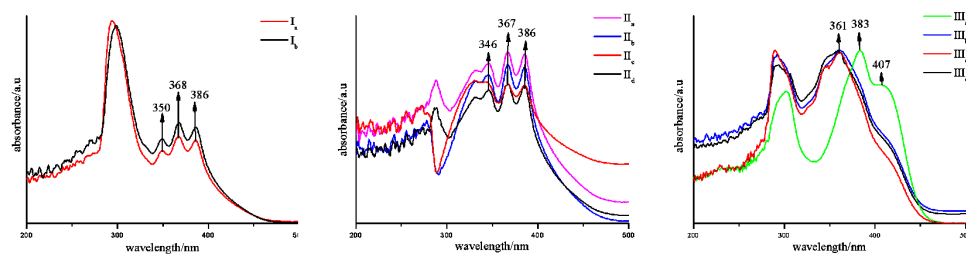
Figure S2. Comparing of PXRD experimental patterns (black) of crystals with simulated patterns (red).



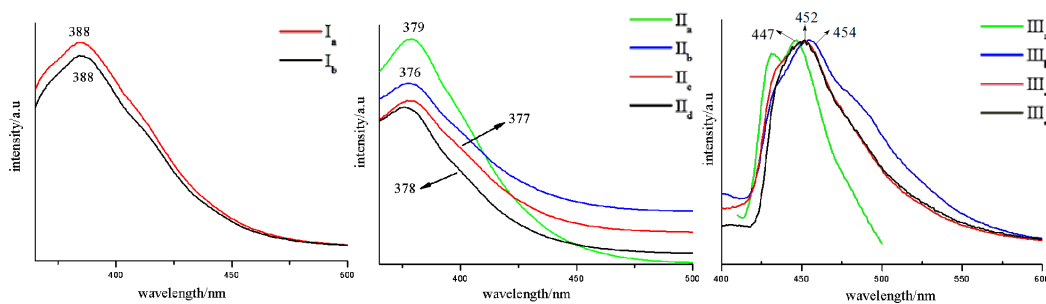
**Figure S3.** DSC measurement for  $\text{II}_a$  and  $\text{II}_c$  investigated by DSC-Q10 at  $10^{\circ}\text{C}/\text{min}$  under liquid nitrogen ( $10\text{ mL}/\text{min}$ )



**Figure S4.** IR spectra of crystals.



**Figure S5.** Absorption spectra of crystals in acetonitrile solvent.



**Figure S6.** Fluorescence spectra ( $\lambda_{\text{exc}}=365\text{ nm}$ ) in cyclohexane solution for all forms.

**Table S1.** Total puckering Amplitude Q value and torsion angles in these forms.

Forms	I <sub>a</sub>	I <sub>b</sub>	II <sub>b</sub>	II <sub>c</sub>	II <sub>d</sub>	III <sub>b</sub>	III <sub>d</sub>
Total puckering Amplitude Q for anthracene or pyrene rings/Å	0.219(8)	0.215(3)	0.142(5)	0.122(8)	0.122(4)	0.050(3)	0.098(5)
O-C(carbonyl)-C-C(ethenyl) torsion angles(°)	9.8(9)	44.5(4)	13.1(5)	-19.8(11)	-13.1(6)	12.8(5)	5.3(7)
C-C(=O)-C-C(ethenyl) torsion angles(°)	-169.2(6)	-137.5(3)	-167.4(3)	159.2(7)	167.1(3)	-165.4(3)	178.9(4)
C-O(methoxy group)-C-C torsion angles(°)	-1.2(8)	2.9(3)	/	/	/	-6.7(4)	-2.3(6)

**Table S1.** Total puckering Amplitude Q value and torsion angles in these forms.**Table S2.** Melting point, enthalpy and decomposition temperature rang of all crystals.

Chalcone	I		II			
	I <sub>a</sub>	I <sub>b</sub>	II <sub>a</sub>	II <sub>b</sub>	II <sub>c</sub>	II <sub>d</sub>
Form						
Melting point / °C	139	167	125	149	147	120,125
Enthalpy/J·g <sup>-1</sup>	63.16	87.55	63.86	73.58	39.12	52.19
Decomposition temperature/ °C	250-380	230-340	230-350	200-300	200-300	230-350

Chalcone	III			
	III <sub>a</sub>	III <sub>b</sub>	III <sub>c</sub>	III <sub>d</sub>
Form				
melting point / °C	147	154	162	150
Enthalpy/J·g <sup>-1</sup>	64.85	66.67	40.83	58.55
Decomposition temperature/ °C	260-370	250-380	320-420	270-380

**Table S3.** The maximum absorption and emission peak of all solids.

Forms	I <sub>a</sub>	I <sub>b</sub>	II <sub>a</sub>	II <sub>b</sub>	II <sub>c</sub>	II <sub>d</sub>	III <sub>a</sub>	III <sub>b</sub>	III <sub>c</sub>	III <sub>d</sub>
$\lambda_{max}^{ab}$ /nm	447	433	485	453	443	455	638	676	570	568
$\lambda_{max}^{em}$ /nm	495	/	545	/	/	501, 526	/	577, 603	/	583