Electronic Supplementary Material (ESI) for Soft Matter.

Transformation Process and Mechanism between the α-Conformation and β-Conformation of Conjugated Polymer PFO in Precursor Solution

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Supporting Information

1. The calculation method of the proportion of β-conformation in PFO solution[1]

The proportion of β-conformation in PFO solution can be calculated according to Lambert-Beer's law (Eq. S2), where c_α and c_β are the concentrations of α-conformation and β-conformation, respectively, A (obtained from experiments) is the absorbency and ε is the absorption coefficient. In UV-vis absorption spectra of PFO solutions, it is difficult to obtain the ε for α-conformation and β-conformation. Thus we used the method of molecular simulation to the absorption spectra to calculate the proportion of $\varepsilon_\beta/\varepsilon_\alpha$.[2]

$$\alpha\% + \beta\% = 1 \qquad \text{(S1)}$$

$$\beta\% = \frac{c_\beta}{c_\beta + c_\alpha} = \frac{A_\beta \times \varepsilon_\alpha}{A_\beta \times \varepsilon_\alpha + A_\alpha \times \varepsilon_\beta} \qquad \text{(S2)}$$

By defining six monomer units as the conjugation length,[3] we optimized the symmetry geometries of PFO chains for the approximate calculation of ε using Density Functional Theory (DFT).[4] To calculate the oscillator strengths (f), Time-Dependent Density Functional Theory (TD-DFT) was used,[5] as this method has been found to give reliable results.[6] DFT and TD-DFT are both with a B3LYP hybrid functional basis set level of 6-31G*.[7] All calculations were performed using the Gaussian 03 package.[6] The oscillator strengths (f) of the two conformations are 4.46 for α-conformation at 386 nm and 4.83 for β-conformation at 437 nm. Thus, the proportion of $\varepsilon_\beta/\varepsilon_\alpha$ can be obtained from Eq. S3 and Eq. S4, where k is a constant and ν is the vibration frequency of two conformations. We can calculate the proportion of β-conformation in each UV-vis absorption spectra of PFO solutions using Eq. S2 and Eq. S4.

$$f = k\int \varepsilon d\nu, \qquad f \propto \varepsilon \qquad \text{(S3)}$$

$$\frac{\varepsilon_\beta}{\varepsilon_\alpha} = \frac{f_\beta}{f_\alpha} = \frac{4.83}{4.46} = 1.08 \qquad \text{(S4)}$$

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2. Light emission spectra of the transformation process from α-conformation to β-conformation

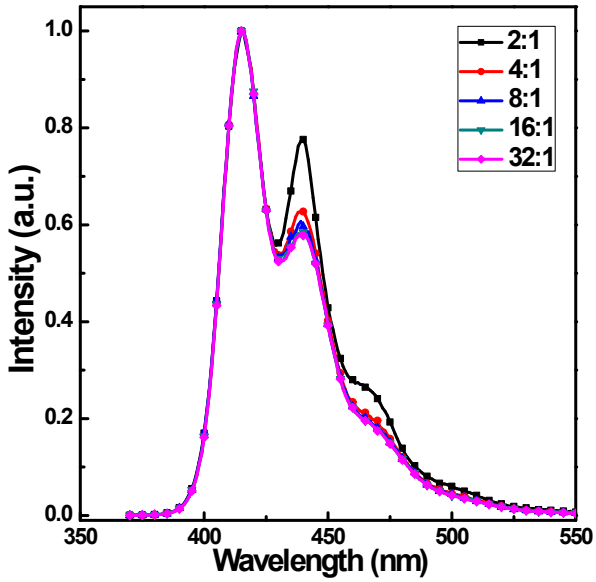

Fig.S1 Normalized light emission spectra of five PFO samples with different toluene/ethanol ratios: 32:1, 16:1, 8:1, 4:1, 2:1. All the five curves were normalized at the 415 nm.

From Fig.S1, it can be seen that the corresponding light emission spectra is well consistent with the UV-vis absorption spectra Fig.2 (a) in the transformation process from α-conformation to β-conformation.