Supporting Information

Study of Chains Condensed Process from Dilute to Concentrated Solution and Chains Conformation's Transformation from Solution to Film for the Conjugated Polymer PFO

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APPENDIX:

1.1 Calculation of the Kuhn length (b) and Kuhn segments (N)

Firstly, R_{max} is the contour length of the PFO chain, R is the Kuhn chain length. According to the previous report, the length of the monomer unit was l = 0.838 nm to the PFO chain, molar mass of the monomer was $M_0 = 390$ g mol⁻¹. Therefore, R_{max} can be calculated as follow: $R_{\text{max}} = \frac{M}{M_0} \times 1 = \frac{127192 \text{ g mol}^{-1}}{390 \text{ g mol}^{-1}} \times 0.838 \text{ nm} = 273 \text{ nm}.$

Then, according to the equation (9) in the main text, the Kuhn segments (*N*) can be calculated as follow: $N = \frac{R_{\text{max}}^2}{R^2} = \frac{273^2}{41.4^2} = 44.$

Finally, according to the equation (10) in the main text, the Kuhn length (b) can be calculated as follow: $b = \frac{R^2}{R_{max}} = \frac{41.4^2}{273} = 6.28 \text{ nm}$

1.2 Calculation of the Kuhn unit relaxation time (τ_0) and Polymer chain relaxation time $(\tau_Z(\tau_R))$

Firstly, $\tau_0 \approx \eta_s b^3 / kT$ is Kuhn unit relaxation time, $k = 1.38 \times 10^{-23}$ J K⁻¹ is the Boltzmann constant, T = 298.15 K is the temperature. In addition, $\eta_s = 4.31 \times 10^{-4}$ (pa·s) is obtained from Figure 1 and b = 6.14 nm is obtained from equation (10) in the main text. Based on the above information, the Kuhn unit relaxation time (τ_0) is calculated as follows:

$$\tau_{0} = \frac{(4.31 \times 10^{-4} \text{ pa} \cdot \text{s}) \times (6.28 \text{ nm})^{3}}{(1.38 \times 10^{-23} \text{ J} \cdot \text{K}^{-1}) \times (298.15 \text{ K})} = \frac{(4.31 \times 10^{-4} \text{ kg} \cdot \text{m}^{-1} \cdot \text{s}^{-1}) \times (6.28 \times 10^{-9} \text{ m})^{3}}{(1.38 \times 10^{-23} \text{ kg} \cdot \text{m}^{2} \cdot \text{s}^{-2} \cdot \text{K}^{-1}) \times (298.15 \text{ K})}$$
$$= \frac{(4.31 \times 10^{-4}) \times (6.28 \times 10^{-9})^{3}}{(1.38 \times 10^{-23}) \times (298.15)} \text{ s} = 2.59 \times 10^{-8} \text{ s}$$

Secondly, according to the equation (1):

$$\tau_{\rm Z} \approx \frac{R^2}{D_{\rm z}} \approx \frac{\eta_{\rm s}}{kT} R^3 = \frac{\eta_{\rm s} b^3}{kT} N^{3\nu} \approx \tau_0 N^{3\nu} \tag{1}$$

Here, $\tau_0 = 2.43 \times 10^{-8}$ s, toluene is the θ solvent of PFO at 25 °C, so, $\nu = 0.5$ can be obtained, and N = 45 is obtained from equation (9) in the main text. Thus, the polymer chain relaxation time (τ_Z) in the Dilute solution is calculated as follows:

$$\tau_Z = (2.59 \times 10^{-8} \text{ s}) \times (44)^{3 \times 0.5} = 7.56 \times 10^{-6} \text{ s}$$

Finally, according to the equation (2):

$$\tau_R \approx \frac{R^2}{D_R} \approx \frac{\zeta}{kT} N R^2 \approx \frac{\eta_s b^3}{kT} N^{1+2\nu} \approx \tau_0 N^{1+2\nu}$$
(2)

Thus, the polymer chain relaxation time (τ_Z) in the Dilute solution is calculated as follows:

$$\tau_R = (2.59 \times 10^{-8} \text{ s}) \times (44)^{1+2 \times 0.5} = 5.01 \times 10^{-5} \text{ s}$$

1.3 GPC experiments

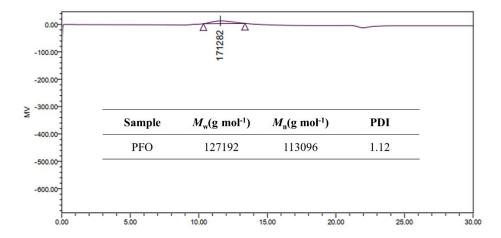


Figure S1. Gel permeation chromatography (GPC) curve, the weight-average molecular weight (M_w), number-average molecular weight (M_n) and the polydispersity index (PDI) of PFO were shown.

1.4 LS experiments

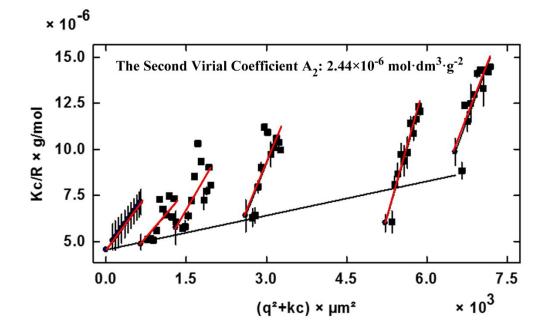


Figure S2 Zimm plots of PFO/toluene dilute solutions at 25 °C.