Supporting Information

Formation of Parallel Aligned Nano-fibrils of Poly(3,3’’’-didodecylquaterthiophene) Induced by the Single Chains in Solution

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The morphology of PQT-12 films with different molecular weight

PQT-12 was fractionized by gradual precipitation.[1] The fractionations formed in a PQT-12 solution in a good solvent with a stepped addition of non-solvent to form precipitations. For example, PQT-12 was first dissolved in THF at a high temperature (90℃). Then the solution was cooled down to room temperature in several minutes, followed by a centrifugation at 9000 rpm for 20 min. After the solid was collected, acetone was added into the remaining solution. Then the solution was heated to 90 ℃, cooled down to room temperature and centrifuged (9000 rpm, 10 min). The solid obtained was collected. Such fractionation process was repeated for several times with increasing the amount of acetone gradually, and then the solids were collected by centrifugation. The M_n and PDI of all fractions were determined by GPC. We named the PQT-12 with different molecular weight as PQT-1# (27 kDa), PQT-2# (21 kDa), and PQT-3# (15 kDa).

TEM was used to observe the differences between their morphologies (Figure S1). PQT-1#, PQT-2#, PQT-3# with a quite similar morphology was observed, which were parallel aligned fibrils. The AFM image (Figure S1c) of PQT-2# (21 kDa) further confirmed the parallel aligned nano-fibrils. At the same time, some rods were found with the parallel fibers. The orientation of these rods was random. The length of these rods was much shorter than the parallel fibrils. PQT-1#, PQT-2#, PQT-3# had diffraction peaks at the same position. (Figure S2)

Figure Captions

Figure S1

TEM images of drop-cast films of PQT-12 with different molecular weights: (a) 26 kDa, (b) 21 kDa, (c) AFM phase image of the PQT-2# (21 kDa) in an area of 2 μm × 2 μm, (d) The TEM image of PQT-2# (15 kDa). The inset is the SAED pattern of the film. All the samples were dissolved in CB with the same concentration of 0.1 mg/mL.

Figure S2

The GI-XRD profile of drop-cast films of PQT-2# with different molecular weights

Figure S3

The chemical structure of PQT-12

Figure S4

The semiquantitative energy schematic of the system. The energy barrier (ΔE_1) of the inter-conversion between unimer coils and aggregates was estimated by Arrhenius equation.

$$\ln(k) = \ln(A) - \frac{E_a}{R}\left(\frac{1}{T}\right) \quad (1)$$

Where k is rate constant (assuming that the solution undergoes the same time to reach equilibrium and using data of different unimer coil population to substitute the rate constant) and pre-exponential factor (A), energy barrier (Ea), gas constant (R), absolute temperature (T). The energy barrier could be estimated by solving these

equations with the different population data (19.9%, 34.5%) at different temperature (274 K, 293 K). The energy barrier E_a is about 21 kJ/mol.

Figure S1

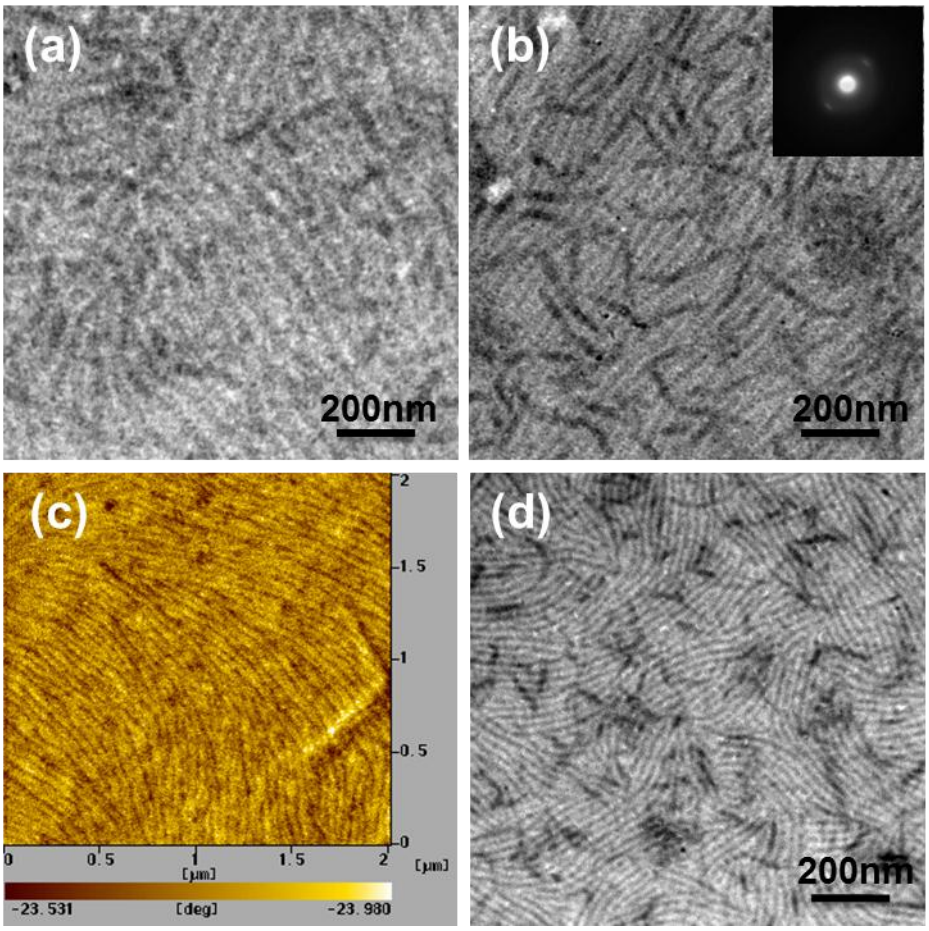


Figure S2

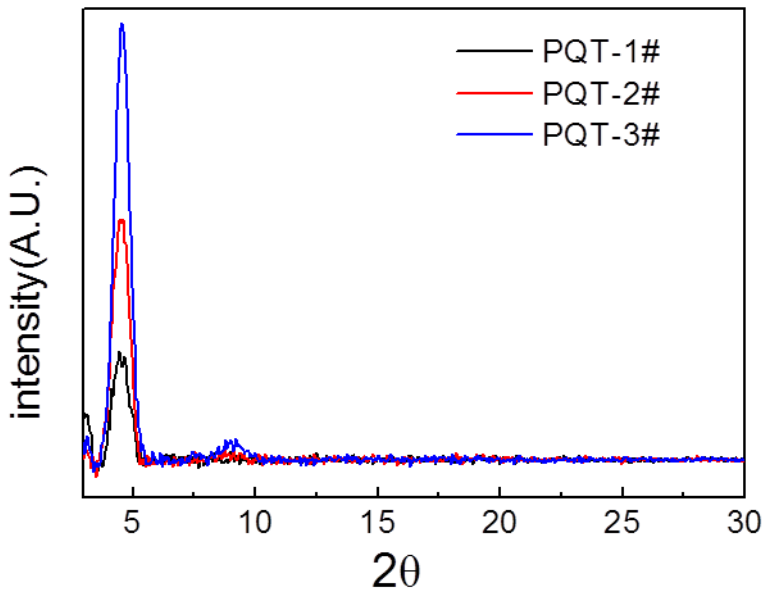


Figure S3

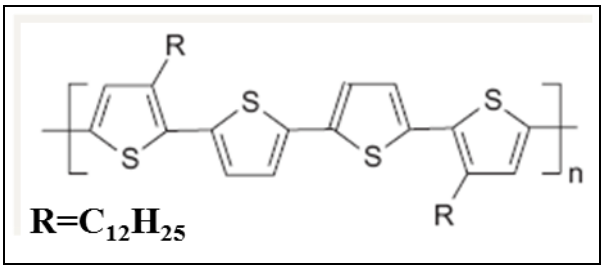
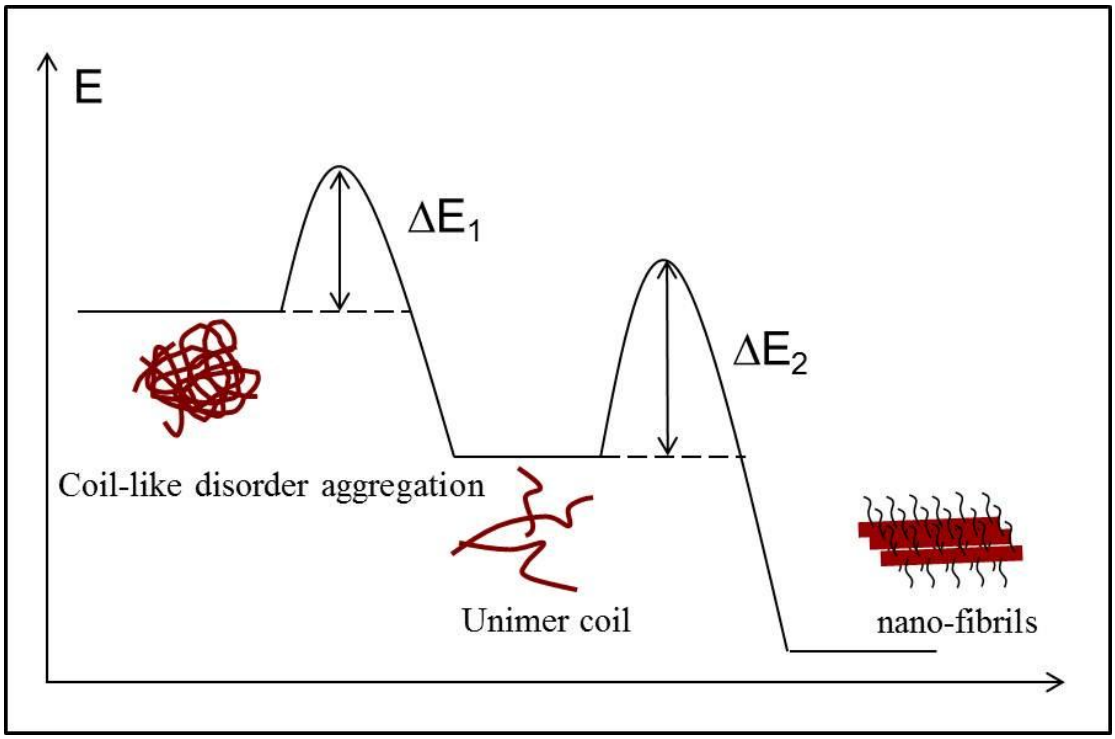


Figure S4



References

[1] J. Liu, I. A. Mikhaylov, J. Zou, I. Osaka, A. E. Masunov, R. D. McCullough, L. Zhai, *Polymer* **2011**, *52*, 2302.