Electronic Supplementary Material (ESI) for Soft Matter.


# Supporting Information

# Understanding of supramolecular solution polymerization and interfacial polymerization via forming multiple hydrogen bonds: a computer simulation study

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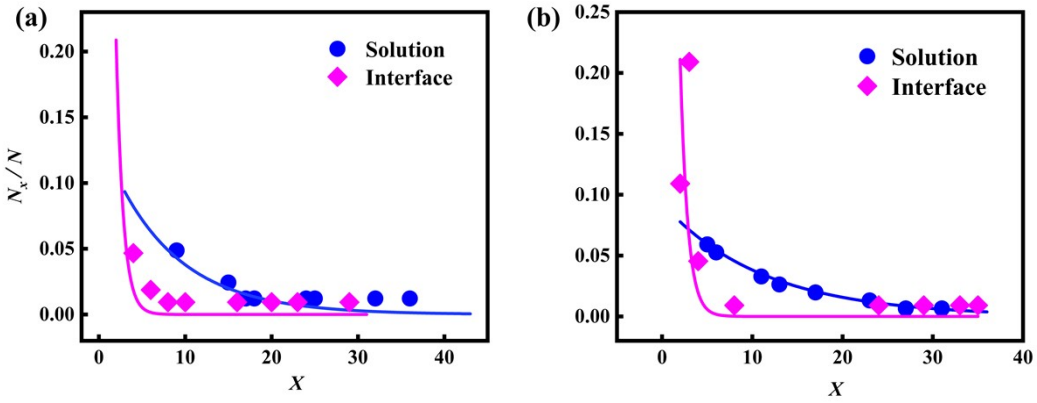


**Figure S1.** Molecular weight distribution of solution polymerization and interfacial polymerization. (a) Triple hydrogen bond model; (b) The sixfold hydrogen bond model. (The Flory distribution formula for linear fitting was used with the same color of the scatters.)

We used the supramolecular model BDB reported by Xing et al. [1]as shown in Figure S2 to carry out simulations. Where the B particles at the end act as the active end groups of the monomer and can react with covalent monomers, and the two middle B-D bonds were non-covalent multiple hydrogen bonds. In our earlier work, we used this model for solution polymerization and interfacial polymerization and the results shown in Figure S3 were obtained via simulation by using the BDB supramolecular model.

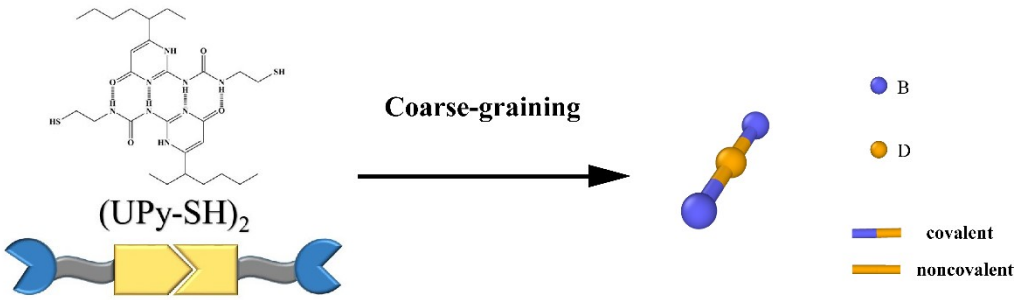


**Figure S2. The simple form (old-version) coarse grained models of supramolecular monomer (Upy-SH)$_2$.**

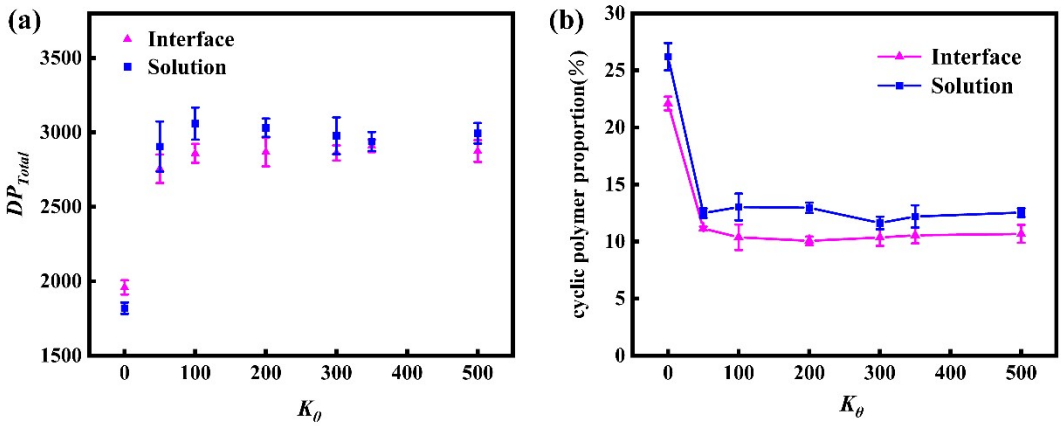


**Figure S3.** (a) Total polymerization degree and (b) cyclic polymer proportion of interfacial polymerization and solution polymerization products under different monomer rigidity.

**References**

1. J.-Y. Xing, Y.-H. Xue, Z.-Y. Lu and H. Liu, *Macromolecules*, 2019, **52**, 6393-6404.