Electronic Supplementary Material (ESI) for Soft Matter.

Supplementary Information: Study of the conformation of polyelectrolyte aggregates using coarse-grained molecular dynamics simulations

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Estimation of the Rigidity of the Fluorocarbon Chain

A full-atom MD simulation of the single $C_{56}F_{114}$ chain is performed for 10^9 steps with $\Delta t = 1$ fs and $T = 300$ K. The TEAM force field software[1] is used to set the parameters for the two-body Lennard-Jones 12-6 potential energy, and three-body and four-body COMPASS-type potential energy[2]. The center of mass of a coarse-grained particle composed of four neighboring carbon atoms and fluorine atoms bonded to the carbon atoms is calculated, and a histogram of the bond angles among three neighboring coarse-grained particles is then monitored. Finally, the histogram is converted into the effective potential energy using the following equation[3]: $U_{\rm eff}(\cos\theta) = -k_{\rm B}T \ln P(\cos\theta)$. Figure S1 shows the effective potential energy, where the minimum value is observed at $\cos\theta = -1$, which corresponds that the bond angle takes $\theta = 180^{\rm o}$ most frequently. The effective potential energy increases with the decrease of the bond angle. The cosine-type potential energy, $U = a(1 + \cos\theta)$ is fitted to the effective potential energy. The prefactor a is estimated to be $4.41 k_{\rm B}T$.

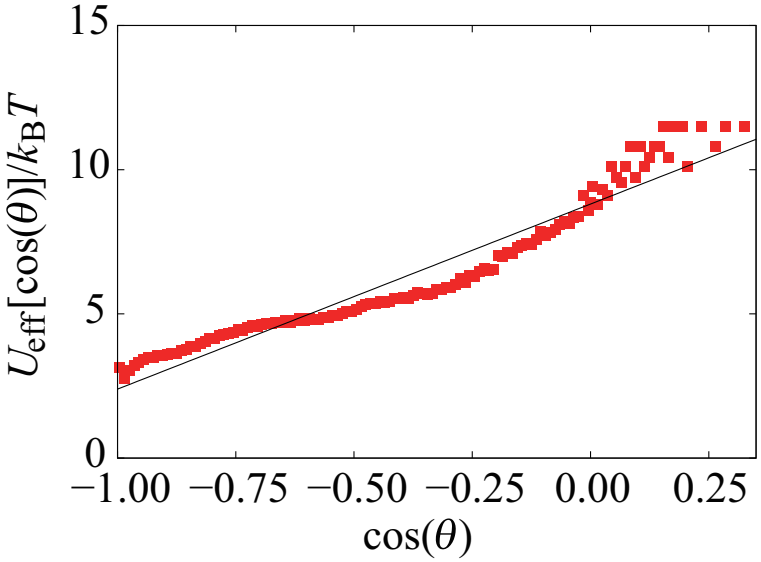

Fig. S1 Effective potential energy of the bond angle among three neighboring coarse-grained particles. The black line represents the fitting function with a prefactor of $4.41 k_{\rm B}T$.

References

1 *Direct Force Field;*, Aeon Technology, Inc.: San Diego, CA 92121.

2 H. Sun, *J. Phys. Chem. B*, 1998, **102**, 7338–7364.

3 V. Harmandaris, N. Adhikari, N. F. van der Vegt and K. Kremer, *Macromolecules*, 2006, **39**, 6708–6719.