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 C56F114 chain is performed for $10^9$ steps with $\Delta t = 1$ fs and $T = 300$ K. The TEAM force field software 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. 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:

$$U_{\text{eff}}(\cos \theta) = -k_B T \ln P(\cos \theta).$$

Figure S1 shows the effective potential energy, where the minimum value is observed at $\cos \theta = -1$, which corresponds that the bond angle takes $\theta = 180^\circ$ 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$k_B T$.

**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$k_B T$.

References

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