Supplementary Information

Atomistic simulation for coil-to-globule transition of poly(2-dimethylaminoethyl methacrylate)

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The potential energy components of PCFF force-field\(^1\) can be defined as follows:

\[
E_{\text{total}} = \sum_{\text{bond } b} \left[ k_2(b - b_0)^2 + k_3(b - b_0)^3 + k_4(b - b_0)^4 \right] + \sum_{\text{angle } \theta} \left[ k_2(\theta - \theta_0)^2 + k_3(\theta - \theta_0)^3 + k_4(\theta - \theta_0)^4 \right] + \sum_{\text{torsion } \phi} \left[ k_1(1 - \cos \phi) + k_2(1 - \cos 2\phi) + k_3(1 - \cos 3\phi) \right] + \sum_{\text{inversion } \chi} K_\chi \chi^2
\]

where the first four components denote the valence interaction, such as bond, angle, torsion, and inversion energy term, the next seven components represent the valence cross-terms, and the last two components are the Coulombic and van der Walls interaction, respectively.

**Figure S1.** Average temperature of (a) PDMAEMA and (b) water molecules during the production run.

**Figure S2.** (a) Equilibrium morphologies of PDMAEMA and (b) time evolution of the radius of gyration for PDMAEMA at 283, 303, and 338 K from the last configuration of the 303 K production run.
**Figure S3.** Time series of the intramolecular pairwise energy of PDMAEMA at 338 K in the extension of the production run.

**Figure S4.** Time evolution of the total system energies at 283, 303, and 338 K.