Electronic Supplementary Material (ESI) for Soft Matter.


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:

$$
\begin{aligned}
E_{total} = & \sum_{bond\ b}\left[k_2(b-b_0)^2 + k_3(b-b_0)^3 + k_4(b-b_0)^4\right] \\
& + \sum_{angle\ \theta}\left[k_2(\theta-\theta_0)^2 + k_3(\theta-\theta_0)^3 + k_4(\theta-\theta_0)^4\right] \\
& + \sum_{torsion\ \phi}\left[k_1(1-cos\phi) + k_2(1-cos2\phi) + k_3(1-cos3\phi)\right] + \sum_{inversion\ \chi} K_\chi \chi^2 \\
& + \sum_{bond\ b}\sum_{bond\ b'} K_{bb'}(b-b_0)\left(b'-b'_0\right) + \sum_{angle\ \theta}\sum_{angle\ \theta'} K_{\theta\theta'}(\theta-\theta_0)\left(\theta'-\theta'_0\right) \\
& + \sum_{bond\ b}\sum_{angle\ \theta} K_{b\theta}(b-b_0)(\theta-\theta_0) + \sum_{bond\ b}\sum_{torsion\ \phi}(b-b_0)(V_1 cos\phi + V_2 cos2\phi + V_3 cos3\phi) \\
& + \sum_{bond\ b'}\sum_{torsion\ \phi}\left(b'-b'_0\right)(V_1 cos\phi + V_2 cos2\phi + V_3 cos3\phi) \\
& + \sum_{angle\ \theta}\sum_{torsion\ \phi}(\theta-\theta_0)(V_1 cos\phi + V_2 cos2\phi + V_3 cos3\phi) \\
& + \sum_{torsion\ \phi}\sum_{angle\ \theta}\sum_{angle\ \theta'} K_{\phi\theta\theta'} cos\phi(\theta-\theta_0)\left(\theta'-\theta'_o\right) + \sum_{i>j}\frac{q_i q_j}{\varepsilon r_{ij}} + \sum_{i>j}\left[\frac{A_{ij}}{r_{ij}^9} - \frac{B_{ij}}{r_{ij}^6}\right]
\end{aligned}
$$

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.

(S1) Sun, H.; Mumby, S. J.; Maple, J. R.; Hagler, A. T. *J. Am. Chem. Soc.* **1994**, *116*, 2978–2987.

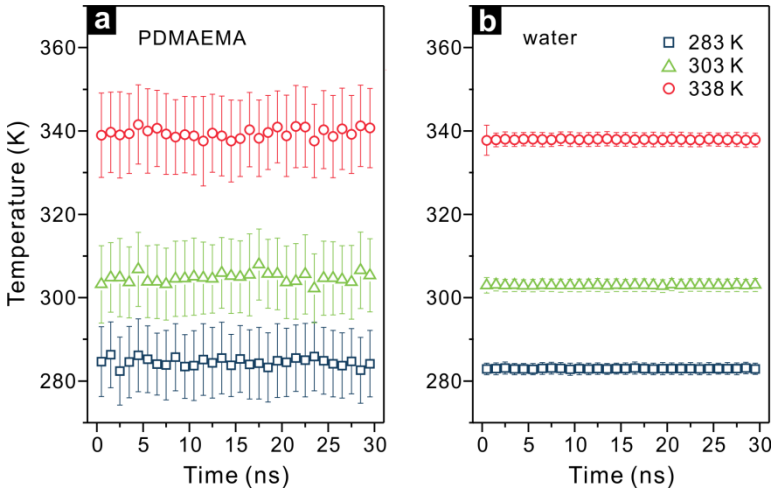


**Figure S1.** Average temperature of (a) PDMAEMA and (b) water molecules during the production run.

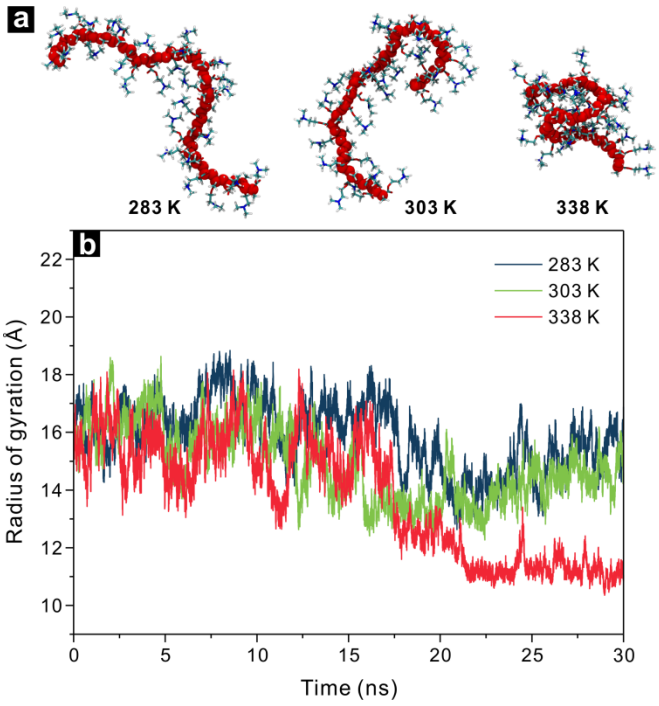


**Figure S2**. (a) Equilibrium morphologies of PDMAEMA and (b) time evolution of the radius of gyration for PDMAEMA at 283, 303, and 338 K from the last configuration of the 303 K production run.

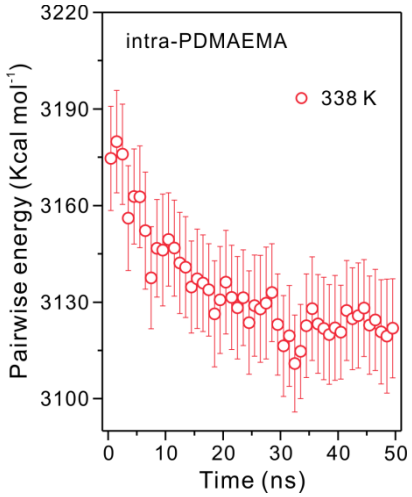


**Figure S3.** Time series of the intramolecular pairwise energy of PDMAEMA at 338 K in the extension of the production run.

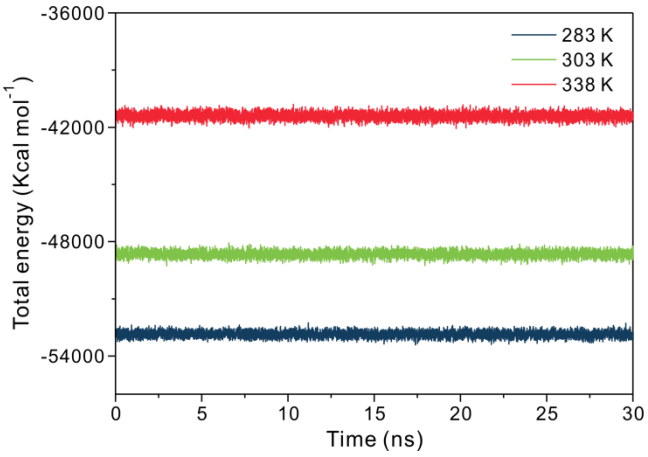


**Figure S4.** Time evolution of the total system energies at 283, 303, and 338 K.