

Electronic Supplementary Information:

Effect of Solvent Quality on the Polymer Adsorption from Bulk Solution onto Planar Surfaces

Per Linse

Physical Chemistry, Department of Chemistry, Lund University
P.O. Box 124, S-221 00 Lund, Sweden

Snapshots displaying the time evolution of the polymer adsorption of the Brownian dynamics simulations are given in Figs. S1–S4 for the four combinations of (i) flexible and (ii) rod-like polymers in (i) good and (ii) theta solvents. In particular, the snapshots display how the initial polymer-free slab at the surfaces are gradually filled with polymers and the conformation of adsorbed polymers given in red.

Furthermore, the equilibrium structure of the adsorbed polymer layer in theta solvent at increasing polymer stiffness is provided in Fig. S5. The nematic ordering with rod-like polymers is clearly visible (bottom left).

Figure Caption

Fig. S1 Snapshots displaying the time evolution with the time given in ns of the polymer adsorption at $k_{\text{angle}} = 0$ (flexible polymers) in a good solvent and $\varepsilon_s = 2.5 \text{ kJ mol}^{-1}$. Beads residing in adsorbed polymers are given in red.

Fig. S2 Snapshots displaying the time evolution with the time given in ns of the polymer adsorption at $k_{\text{angle}} = 30 \text{ J mol}^{-1} \text{ deg}^{-2}$ (rod-like polymers) in a good solvent and $\varepsilon_s = 2.5 \text{ kJ mol}^{-1}$. Beads residing in adsorbed polymers are given in red.

Fig. S3 Snapshots displaying the time evolution with the time given in ns of the polymer adsorption at $k_{\text{angle}} = 0$ (flexible polymers) in a theta solvent and $\varepsilon_s = 2.5 \text{ kJ mol}^{-1}$. Beads residing in adsorbed polymers are given in red.

Fig. S4 Snapshots displaying the time evolution with the time given in ns of the polymer adsorption at $k_{\text{angle}} = 30 \text{ J mol}^{-1} \text{ deg}^{-2}$ (rod-like polymers) in a theta solvent and $\varepsilon_s = 2.5 \text{ kJ mol}^{-1}$. Beads residing in adsorbed polymers are given in red.

Fig. S5 (left) Perspective and (right) side view of snapshots displaying one surface with adsorbed polymers from the final equilibrium configuration at (top to bottom) $k_{\text{angle}} = 0$ (flexible polymers), $k_{\text{angle}} = 1.2 \text{ J mol}^{-1} \text{ deg}^{-2}$ (semi-flexible polymers), $k_{\text{angle}} = 10 \text{ J mol}^{-1} \text{ deg}^{-2}$ (stiff polymers), and $k_{\text{angle}} = 30 \text{ J mol}^{-1} \text{ deg}^{-2}$ (rod-like polymers); all in a theta solvent and at $\varepsilon_s = 2.5 \text{ kJ mol}^{-1}$.

Figure S1 (flexible polymer, good solvent)

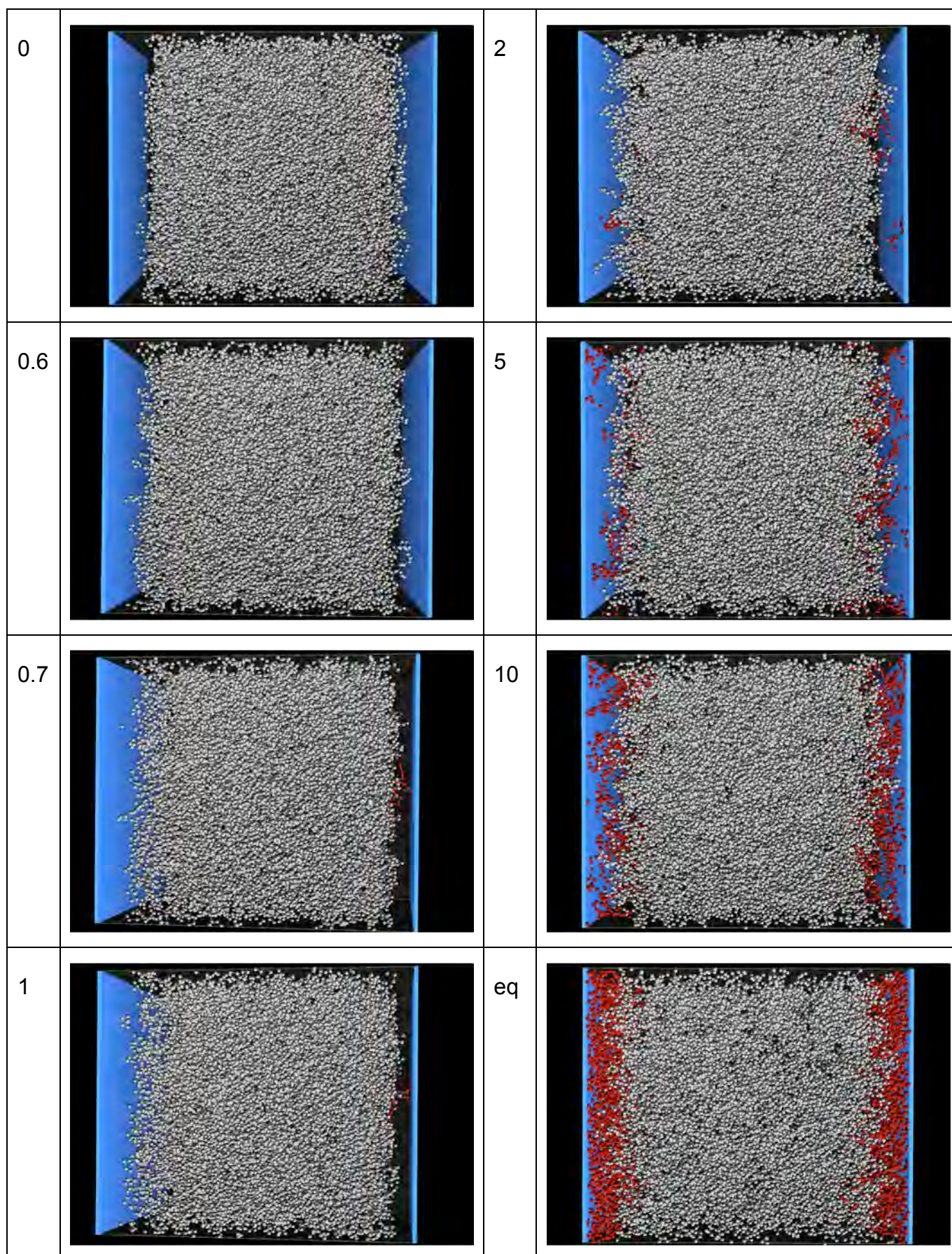


Figure S2 (rod-like polymer, good solvent)

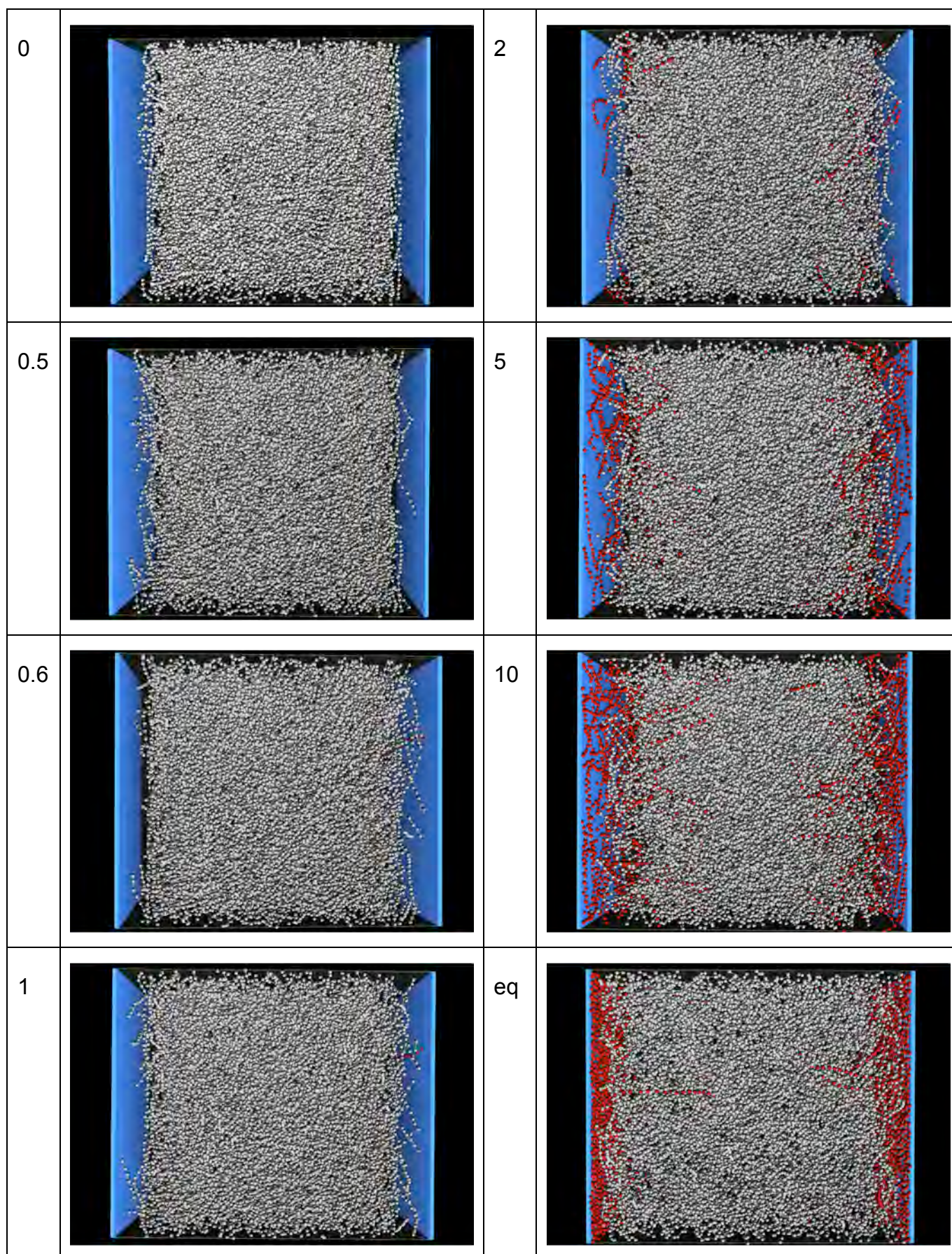


Figure S3 (flexible polymer, theta solvent)

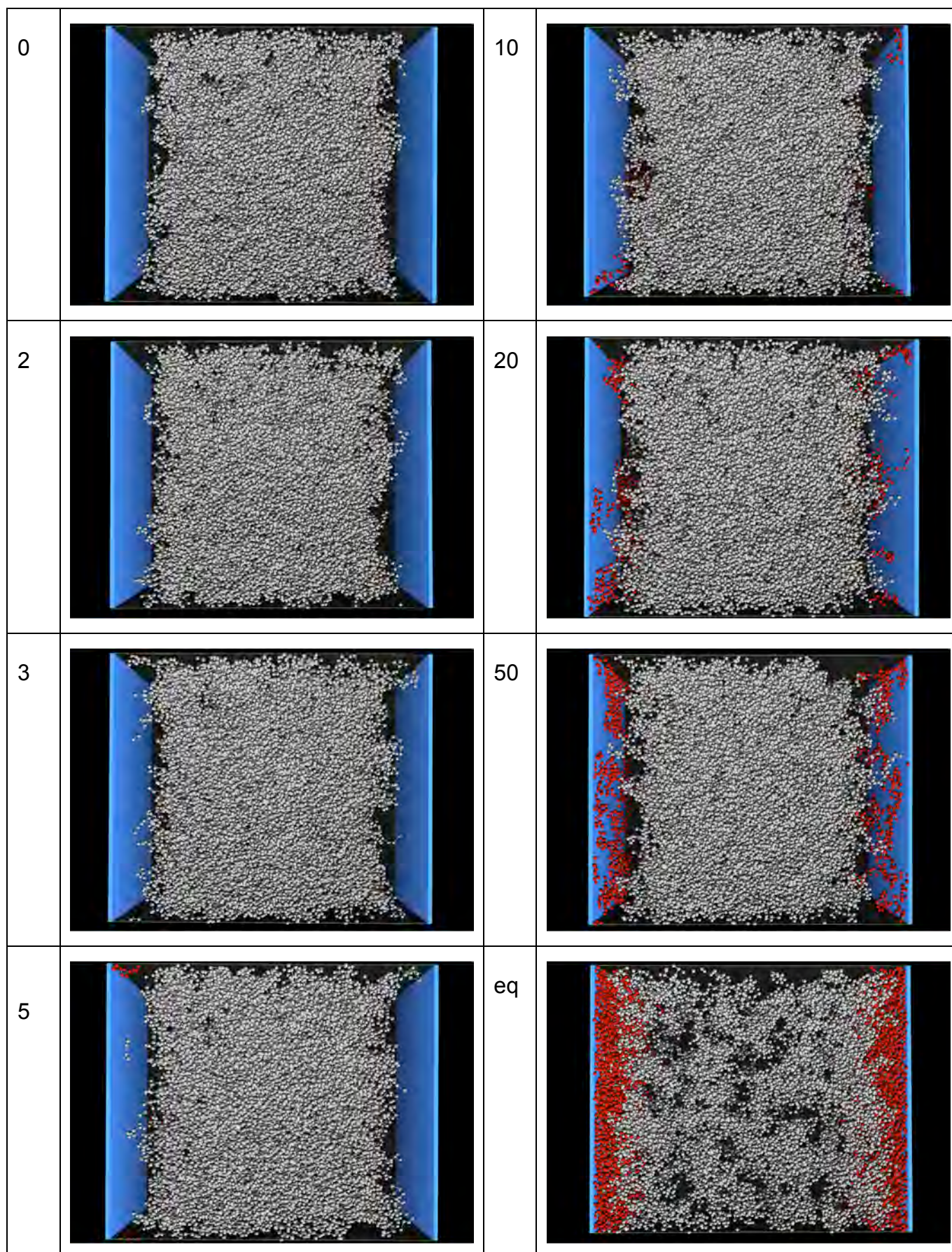
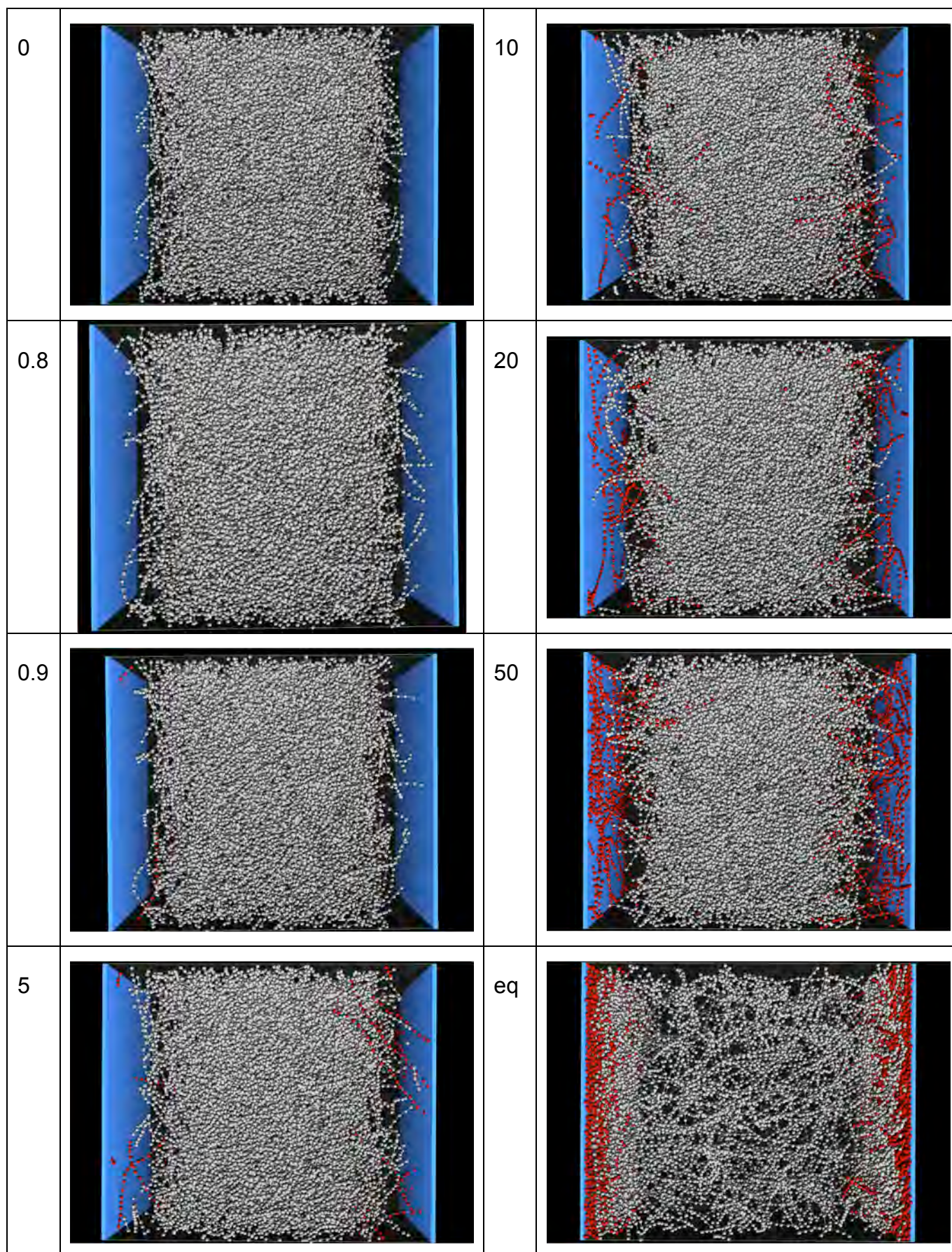


Figure S4 (rod-like polymer, theta solvent)



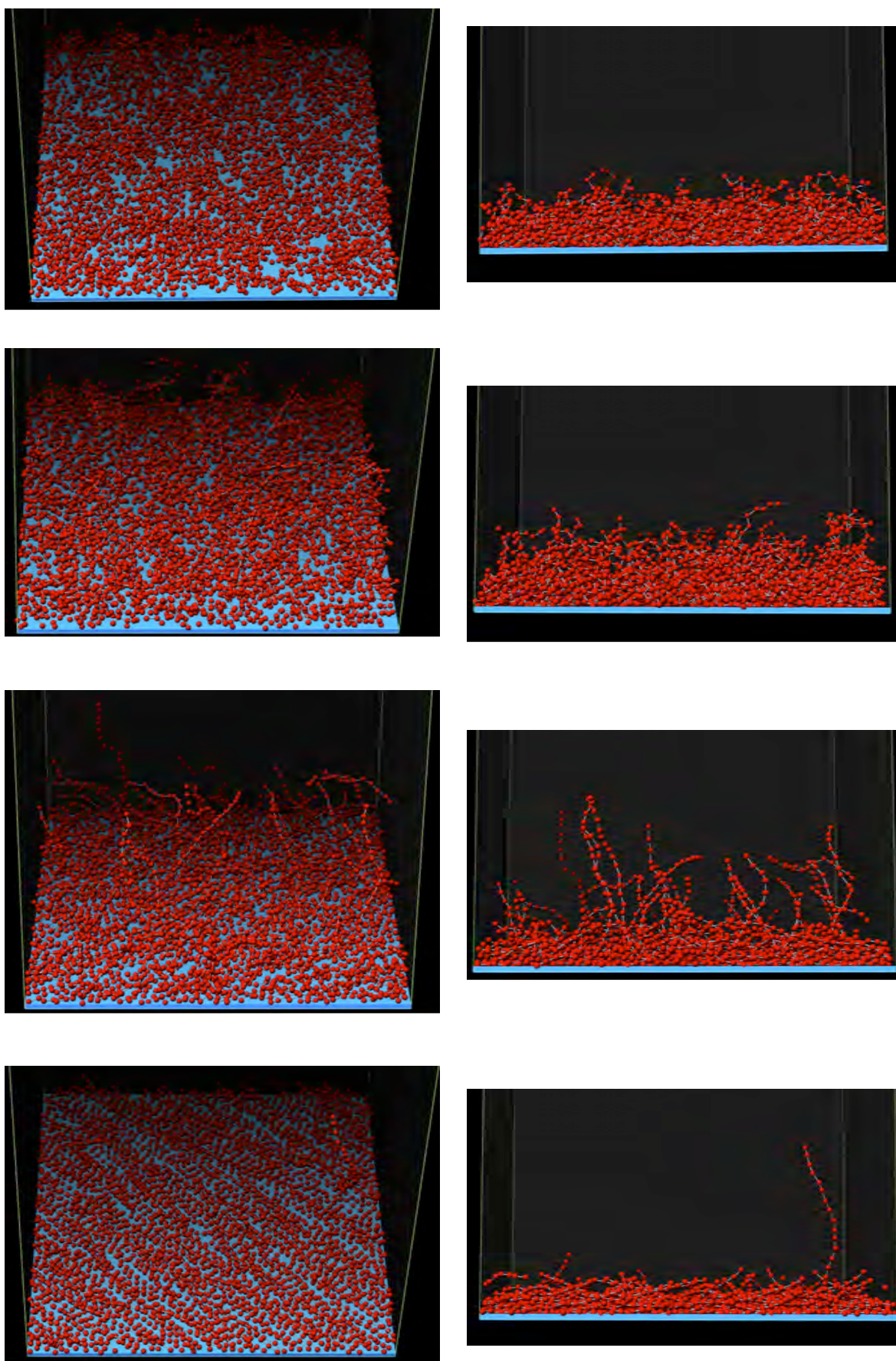


Figure S5