Supplementary Information

Crowding-induced interactions of ring polymers

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1 Methods

Umbrella sampling for polymer-polymer interactions

We performed umbrella sampling along the distance between the centers of mass of two ring polymers. For $\phi \geq 0.2$, we sampled from a distance of 3σ to a distance of 13σ with a step size of 0.5σ between the centers of the biasing potentials. For $\phi = 0$ and 0.1, we sampled until 15σ. The simulation box was periodic in all dimensions with box size of $30\sigma \times 30\sigma \times 30\sigma$ for all crowding fractions for $\phi \geq 0.2$. For $\phi = 0$ and 0.1, the box size was $40\sigma \times 40\sigma \times 40\sigma$. In the bias potential $U_{\text{bias}} = \frac{1}{2}k(r_{12}^0 - r_{12})^2$, the force constant k was set to ϵ/σ^2.

For each window considered, simulations were run for a total of 5×10^7 timesteps, with timestep $\Delta = 0.005\tau$. The production run for each window was obtained after 7.5125×10^6 equilibration timesteps. Histograms of the distances sampled in each window are shown in Fig. S2 below. In the Weighted Histogram Analysis Method (WHAM), we used a bin width of 0.1σ and a convergence tolerance of 10^{-6} for the iterations.

Umbrella sampling for polymer-wall interactions

We performed umbrella sampling along the distance between the center of mass of a ring polymer and a fixed wall. The simulation box was 30σ in the z direction (normal to the wall) and 25σ in the x and y directions. Table S1 below provides the parameter values used for the umbrella sampling for different crowding fractions. We limited our umbrella sampling to crowding fractions $\phi \leq 0.25$.

For each window considered, simulations were run for a total of 5×10^7 timesteps, with timestep $\Delta = 0.005\tau$. The production run for each window was obtained after 1.5×10^7 equilibration timesteps. Histograms of the distances sampled in each window are shown in Fig. S3 below. In WHAM, we used a bin width of 0.1σ and a convergence tolerance of 10^{-6} for the iterations.

For the umbrella potentials, larger force constants were used to study the polymer-wall interactions compared with the polymer-polymer case. This was due to the strong effective interactions between the polymer and wall at small distances. Using the strong biasing potential, we obtained good sampling of distances for the entire range of z_{pw}, as shown in Fig. S3.

2 Supplemental figures and table

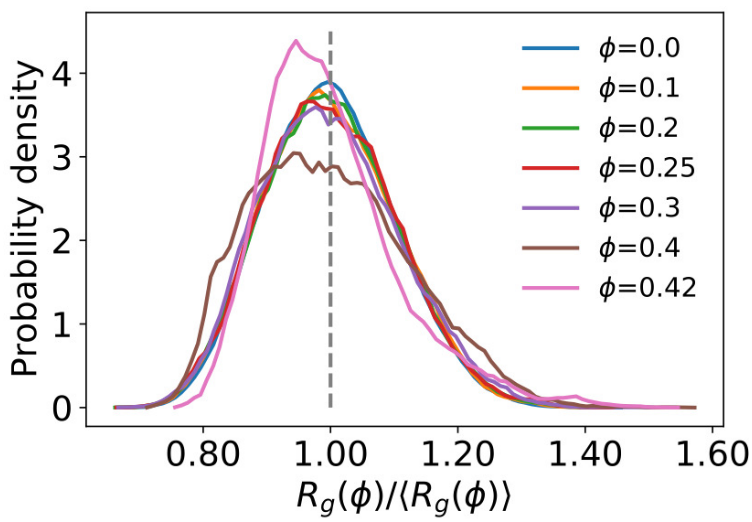

Figure 1: For an isolated ring polymer, the probability density of the radius of gyration ($R_g(\phi)$) scaled by the average radius of gyration ($\langle R_g(\phi)\rangle$). Distributions are shown for different crowding fractions (ϕ).

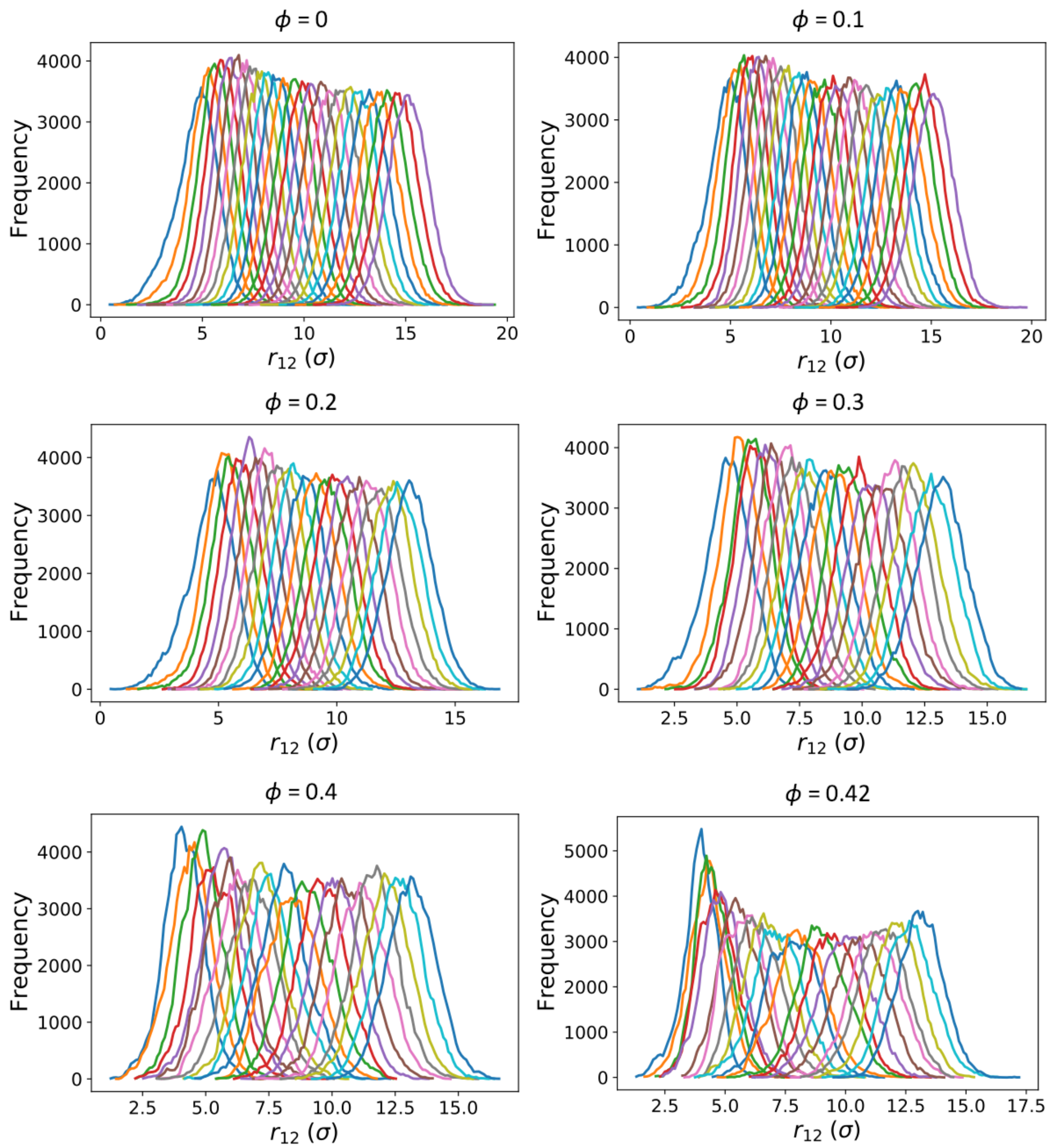

Figure 2: Umbrella sampling for polymer-polymer interactions: Histograms of distances between the centers of mass (r_{12}) observed in each sampling window at different crowding fractions (ϕ).

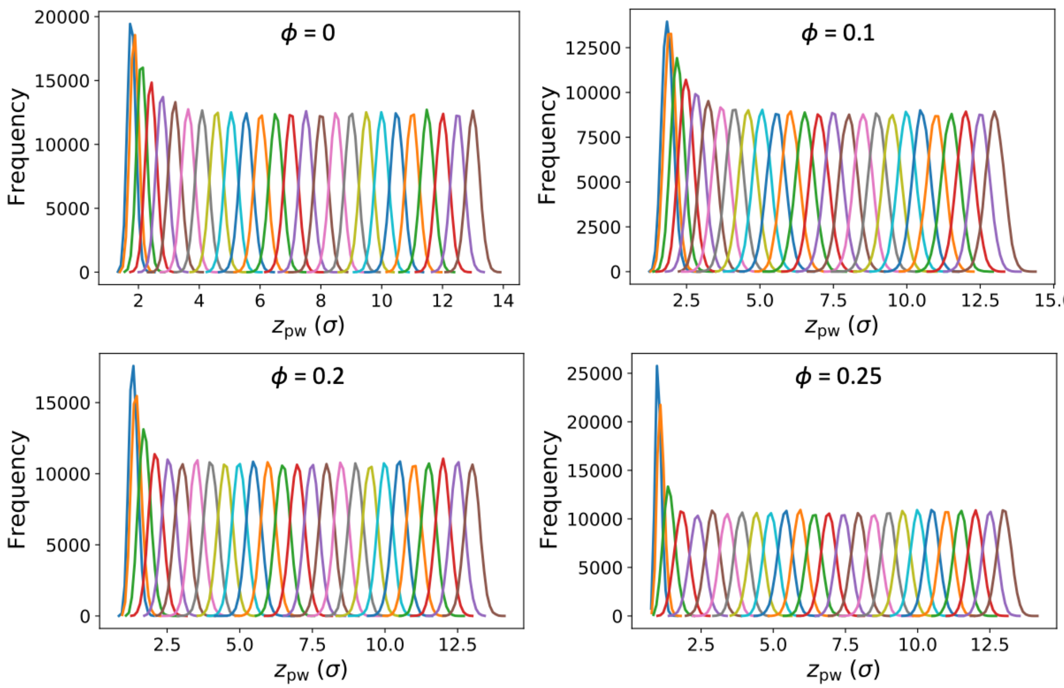

Figure 3: Umbrella sampling for polymer-wall interactions: Histograms of distances between the polymer's center of mass and the wall (z_{pw}) observed in each sampling window at different crowding fractions (ϕ).

Table 1: Parameters for umbrella sampling along the distance between the center of mass of the polymer and the wall. The biasing potential was $U_{\text{bias}} = \frac{1}{2}k(z_{pw}^0 - z_{pw})^2$.

$\phi = 0.0$

$z_{pw}^0(\sigma)$	$k\ (\epsilon/\sigma^2)$
0.75	20.00
1.00	20.00
1.50	20.00
2.00	20.00
2.50	20.00
3.00	20.00
3.50	20.00
4.00	20.00
4.50	20.00
5.00	20.00
5.50	20.00
6.00	20.00
6.50	20.00
7.00	20.00
7.50	20.00
8.00	20.00
8.50	20.00
9.00	20.00
9.50	20.00
10.00	20.00
10.50	20.00
11.00	20.00
11.50	20.00
12.00	20.00
12.50	20.00
13.00	20.00

$\phi = 0.1$

$z_{pw}^0(\sigma)$	$k\ (\epsilon/\sigma^2)$
0.75	10.00
1.00	10.00
1.50	10.00
2.00	10.00
2.50	10.00
3.00	10.00
3.50	10.00
4.00	10.00
4.50	10.00
5.00	10.00
5.50	10.00
6.00	10.00
6.50	10.00
7.00	10.00
7.50	10.00
8.00	10.00
8.50	10.00
9.00	10.00
9.50	10.00
10.00	10.00
10.50	10.00
11.00	10.00
11.50	10.00
12.00	10.00
12.50	10.00
13.00	10.00

$\phi = 0.2$

$z_{pw}^0(\sigma)$	$k\ (\epsilon/\sigma^2)$
0.75	25.00
1.00	25.00
1.50	15.00
2.00	15.00
2.50	15.00
3.00	15.00
3.50	15.00
4.00	15.00
4.50	15.00
5.00	15.00
5.50	15.00
6.00	15.00
6.50	15.00
7.00	15.00
7.50	15.00
8.00	15.00
8.50	15.00
9.00	15.00
9.50	15.00
10.00	15.00
10.50	15.00
11.00	15.00
11.50	15.00
12.00	15.00
12.50	15.00
13.00	15.00

$\phi = 0.25$

$z_{pw}^0(\sigma)$	$k\ (\epsilon/\sigma^2)$
0.75	25.00
1.00	25.00
1.25	25.00
1.50	15.00
2.00	15.00
2.50	15.00
3.00	15.00
3.50	15.00
4.00	15.00
4.50	15.00
5.00	15.00
5.50	15.00
6.00	15.00
6.50	15.00
7.00	15.00
7.50	15.00
8.00	15.00
8.50	15.00
9.00	15.00
9.50	15.00
10.00	15.00
10.50	15.00
11.00	15.00
11.50	15.00
12.00	15.00
12.50	15.00
13.00	15.00