Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information
Mapping a single-molecule folding process onto a topological space

Maziar Heidari,[1,2] Vahid Satarifard,[1,3] and Alireza Mashaghi[1]

[1] *Leiden Academic Centre for Drug Research, Faculty of Mathematics and Natural Sciences, Leiden University, Leiden, The Netherlands*
[2] *Max Planck Institute for Polymer Research, Mainz, Germany*
[3] *Max Planck Institute of Colloids and Interfaces, Potsdam, Germany*

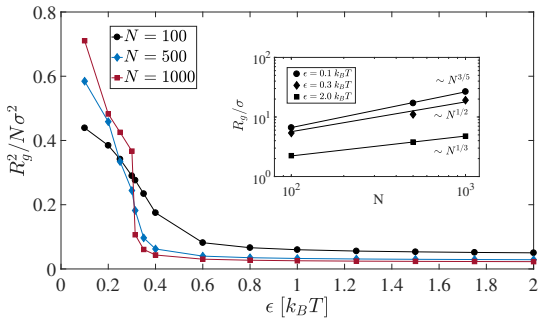

FIG. 1. Normalized squared radius of gyration of LJ chains $R_g^2/N\sigma^2$ is shown against different cohesive strength ϵ. Inset shows the radius of gyration against number of monomers. Lines represent scaling fit to the data points. The radius of gyration of a polymer having N monomers is calculated by $R_g^2 = \frac{1}{N}\sum_{k=1}^{N}(\mathbf{r}_k - \mathbf{r}_m)^2$. Here, $\mathbf{r}_m = 1/N\sum_k \mathbf{r}_k$ is the mean position of the monomers

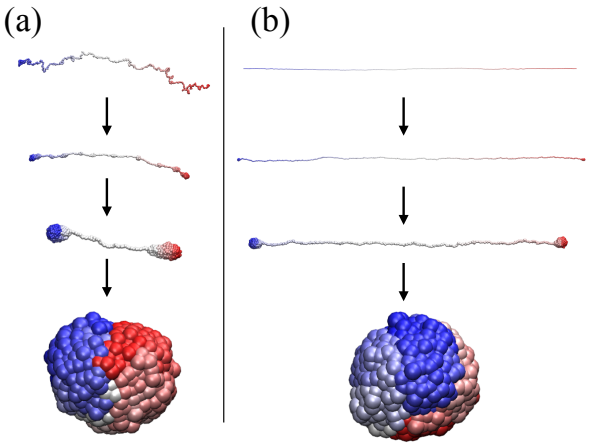

FIG. 2. Snapshots of the free chain in the course of simulation time when the initial condition of the chain is a coiled structure (a) or a fully stretched conformation (b).

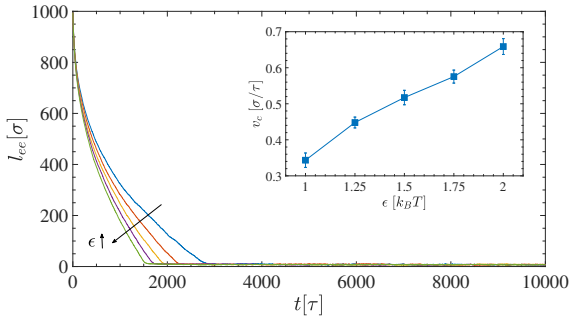

FIG. 3. Time series of the end-to-end distance (l_{ee}) of a FSC for different cohesive strength (ϵ). In all cases, the chain is initially in the fully extended state ($l_{ee} = 1000\sigma$). Inset shows the folding speed of the chain against different cohesive strength. The averages and error bars are obtained from ten independent simulation runs by linearly fitting to the chain's length-time data.

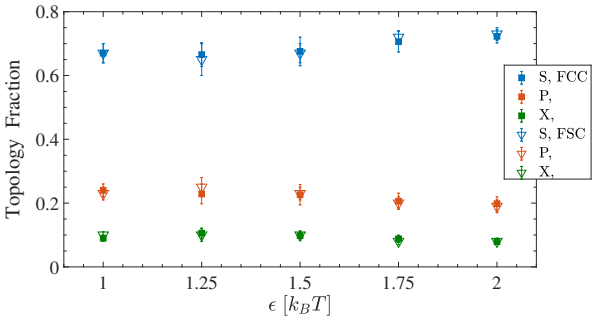

FIG. 4. Topology fractions of series (S), parallel (P) and cross (X) loops of globules against cohesive interaction ϵ. The globules are obtained from simulations of free chains having coiled (FCC) and stretched (FSC) initial conditions. The averages and error bars are calculated over 10 independent trajectories.

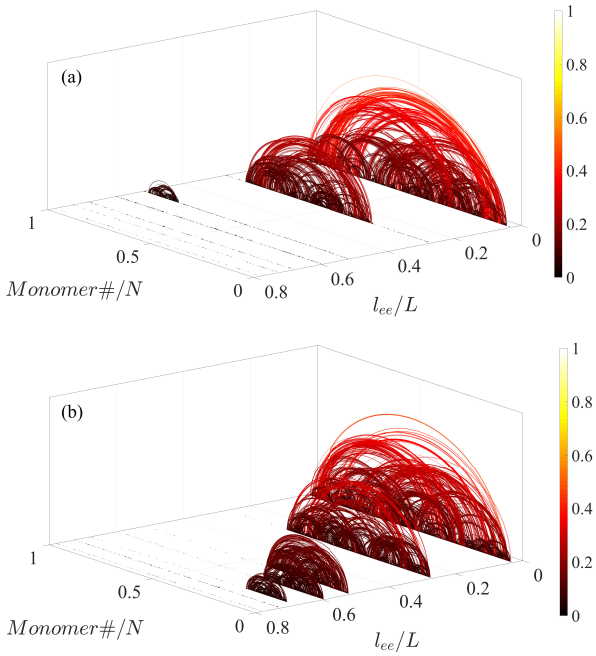

FIG. 5. The loop distributions along the chain when the chain is folded. Each semi-circle connecting two monomers represents a contact. The folding speed is $v_f = 1 \times 10^{-3}\sigma/\tau$ and the cohesive strength is $\epsilon = 1.0k_BT$ (a) and $\epsilon = 2.0k_BT$ (b). The color bar shows the size of the loops normalized to the contour length of the chain.

$\epsilon\ [k_BT]$	1.0	1.25	1.5	1.75	2.0
γ_V	11.6	12.5	13.1	13.5	12.9
γ_S	-27.2	-28.2	-28.8	-27.2	-26.1

TABLE I. The parameters obtained from fitting Eq. 5 to the internal energy of the globules with different cohesive strength (ϵ).

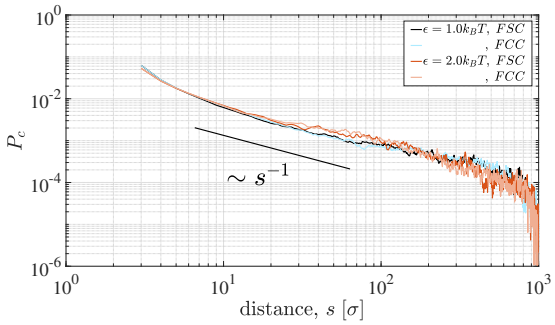

FIG. 6. The probability of contacts of FCC and FSC as a function of distance s for different globules. The contact probability in all globules decay with scaling $\sim s^{-1}$ within the intermediate distance interval. All curves are obtained through averaging over final configurations of 10 independent simulation runs.

$k_BT \times 10^{-3}$	a_0	a_2	a_4	a_6	a_8
IC	-4.3443	0.6758	6.8573	-14.3201	11.1403
SAC	-4.1545	-0.5573	9.7969	-17.3532	12.2817

TABLE II. The parameters obtained by fitting Eq. 9 of the main text to free energy obtained from contraction experiment.