

Can comb copolymers be used as molecular switches ?

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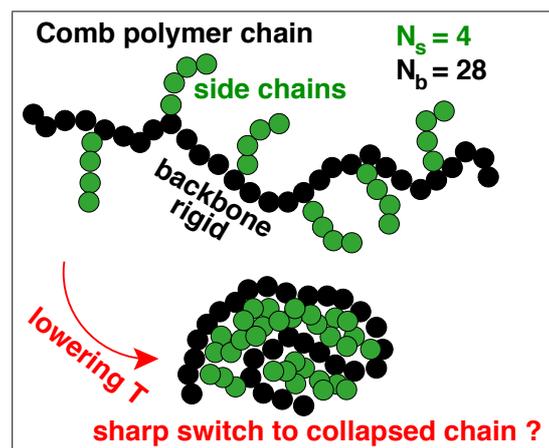
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Research context:

Our research group at the ICS is interested quite generally in the statistical physics of soft matter and the rheology of complex fluids with a particular emphasis on systems involving polymers [1]. Using simple coarse-grained models many fundamental and generic aspects of such systems can be investigated by means of Monte Carlo (MC) or molecular dynamics simulations [2-4]. Motivated by recent experimental work on surprisingly stable freestanding thin films of copolymer melts far from the glass transition [5] a new research axis in our group is concerned with the numerical simulation and analysis of comb copolymers.

Project description:

We propose a simple “how-to-do-it” tutorial example of a molecular dynamics simulation study of a single polymer chain using a standard bead-spring model [1]. As shown in the figure we shall compute comb polymers with a relatively rigid backbone which at high temperatures assumes an open, elongated linear shape. While decreasing the temperature the chain should collapse due to the attraction of the side chains. The question is of whether it is possible to tune the parameters of the model such that the transition becomes very sharp allowing thus to use comb polymers as molecular switches.



Required tasks and workflow:

1. Get acquainted to the LAMMPS code [4];
2. Create one single comb chain ($M_c = 1$) of backbone length $N_b = 64$ with $M_s = 8$ short side chains of length $N_s = 8$;
3. Let us assume a relatively rigid backbone and purely repulsive interactions. Create an ensemble of $m = 100$ independent equilibrated chains at a temperature $T = 1$. Perform then production runs (time series) over the ensemble.
4. Compute static properties such as the radius of gyration or the static structure factor [1] of the total chain, its backbone and its side chains;
5. Compute mean-square displacements, reorientation correlation function and from this the relaxation time and diffusion coefficient;
6. Let us then switch on the attractive part of the LJ interactions. How do static and dynamical properties change ?

7. Decrease the temperature. Do you observe a chain collapse for low temperatures ? Can this transition be made sharper by tuning the parameters N_b , N_s or M_s ?
8. Preparation of internship report and talk.

References:

- [1] M. Rubinstein and R.H. Colby, *Polymer Physics*, Oxford University Press (2003).
- [2] M.P. Allen and D.J. Tildesley, *Computer Simulation of Liquids*, Oxford University Press (1994).
- [3] D. Frenkel and B. Smit, *Understanding Molecular Simulation – From Algorithms to Applications*, Academic Press, San Diego (2002).
- [4] S. J. Plimpton, *Fast Parallel Algorithms for Short-Range Molecular Dynamics*, J. Comp. Phys. **117**, 1 (1995).
- [5] T. Gaillard *et al.*, *Stable freestanding thin films of copolymer melts far from the glass transition*, MacroLetters, **4**, 1144 (2015).