Active Hydrogels – Simulations

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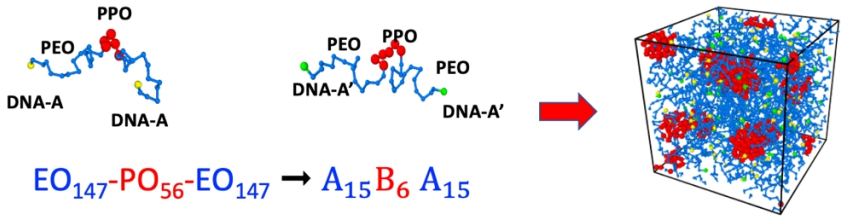

Motivation

Hydrogels are solid materials predominantly made of water and a small fraction of self-assembled polymers. In everyday live we encounter hydrogels in form of foods, cosmetics and care products. But they are also essential in applications such PCR tests, we had to go through in the past 3 years and DNA testing, pharmaceutics and diagnostic tools. Here we are interested in the study of hydrogels made of symmetric, non-ionic triblock-copolymers, which are known as Pluronics®. At low temperatures their aqueous solutions are liquid. However, upon heating water becomes a less good solvent for the middle block and the chains start to aggregate to form micelles as shown in the simulation snaphot above[1]. At sufficiently high concentrations the micelles form a soft, gel-like crystal. By adding smart overhands, for instance short, single-stranded DNA, such systems can be made 'active', meaning they will react to an external stimulus.

Your Project

In this project the student will familiarize themselves with a Molecular Dynamics model of these triblock-copolmers, previously mapped onto the real system[1], in LAMMPS[2]. As first task the student will perform some tests like, checking the self-assembling behaviour and reproduce a few points in the systems phase diagram[3]. The challenge will be to model the appropriate interactions between the free chain ends in terms of sticky patches with appropriate interaction potentials that will lead to the systems gelation in prescribed parameter settings. If time permits the structure and assembling dynamics will be explored.

Requirements

Background in Soft Matter physics would be advantageous. We would like an applicant who is interested in numerical model.

Other aspects

The project will be supervised by the Professor Eiser, an expert in the rheology of self-assembling DNA systems. Associate Professor Cabriolu is an expert in simulation studies of soft matter systems. If interested the student can do both simulations and experiments.

[1] Jiaming Yu - PhD thesis: https://www.repository.cam.ac.uk/handle/1810/345675 (2023)
[2] LAMMPS Molecular Dynamics Simulator: https://www.lammps.org/#gsc.tab=0
[3] R. Liu, A. Caciagli, J. Yu, X. Tang, R. Ghosh, E. Eiser 'Dynamic Light Scattering based microrheology of End-functionalised triblock copolymer solutions' *Polymers* **15**, 481 (2023)