CPP 34: Hydrogels and Microgels

Time: Thursday 9:30–10:15 Location: H39

CPP 34.1 Thu 9:30 H39

Simulations explain the Swelling Behavior of Hydrogels with Alternating Neutral and Weakly Acidic Blocks — •David Beyer[1], Peter Košovan[2], and Christian Holm[1] — [1]Institute for Computational Physics, University of Stuttgart, D-70569 Stuttgart, Germany — [2]Department of Physical and Macromolecular Chemistry, Charles University, Prague, Czechia

We use computer simulations to study a coarse-grained model of a weak (pH-responsive) polyelectrolyte hydrogel which consists of a covalent, regular tetra-functional network of four-armed neutral and acidic stars, coupled to a reservoir of small ions. A similar system consisting of tetrapoly-(acrylic acid) and tetrapoly(ethylene glycol) was recently investigated experimentally by the Sakai group. To model the ionization equilibrium of the weak groups and the exchange of small ions with the reservoir, we make use of the recently developed Grand-Reaction Monte-Carlo method (G-RxMC). We determine the free swelling equilibrium for different salt concentrations and pH values of the reservoir. The results for the swelling ratio are in good agreement with the experimental data for high and intermediate pH values. We obtain titration curves which display a significant deviation from the ideal Henderson-Hasselbalch equation due to charge correlations and Donnan partitioning. Contrary to a previous conjecture, our results show that counterion condensation does not explain the observed swelling behavior. Finally, we investigate the gel structure and observe that the swelling is dominated by the stretching of the acidic blocks.

CPP 34.2 Thu 9:45 H39

Importance of pH in Synthesis of pH-Responsive Cationic Nano- and Microgels — •Marco Annegarn, Maxim Dirksen, and Thomas Hellweg — Department of Physical and Biophysical Chemistry, Bielefeld University, Universitätsstraße 25, 33615 Bielefeld, Germany

While cationic nano- and microgels are potentially useful for transfection of cells or the immobilization of biomacromolecules, their synthesis often has certain drawbacks regarding size, polydispersity, yield and incorporation of the cationic comonomer. Since many cationic comonomers like primary or secondary amines are pH-responsive, their charge relies on the surrounding pH. Therefore, a range of poly(*N*-isopropylacrylamide) (PNIPAM) microgels with the primary amine *N*-(3-aminopropyl)methacrylamide hydrochloride (APMH) as the cationic comonomer were synthesized at different reaction pH. The microgels were analyzed with respect to their size, thermoresponsive swelling behavior, synthesis yield, polydispersity and APMH-incorporation.

The results show that the reaction pH has a strong influence on on all the mentioned parameters and can be utilized to tailor the microgels properties. While the influence of the pH on such microgels has been examined repeatedly after synthesis, the influence of the reaction pH during synthesis is mostly ignored. Hence, a precise pH-control during the synthesis of microgels with pH-responsive moieties is crucial to gain reproducible and comparable results.

CPP 34.3 Thu 10:00 H39

Behaviour of a magnetic nanogel in a shear flow — •Ivan Novikau[1], Ekaterina Novak[2], Elena Pyanzina[2], and Sofia Kantorovich[1,2] — [1]University of Vienna, Austria — [2]Russia

Magnetic nanogels (MNG) are promising magneto-controllable drug carriers. In order to develop this potential, one needs to study MNG's behavior in various microfluidic systems, one of which can be modelled as a channel with a given flow.

Considering the size of the MNG and typical time and velocity scales involved in their nanofluidics, experimental characterisation of the system is challenging. In this work, we perform molecular dynamics (MD) simulations combined with the Lattice-Boltzmann (LB) scheme aiming at describing the impact of the shear rate on the shape, magnetic structure and motion of an MNG.

We find that in a shear flow, the centre of mass of an MNG tends to be in the centre of a channel and to move, preserving the distance to both walls. The MNG monomers along with translation are involved in two more types of motion, they rotate around the centre of mass and oscillate with respect to the latter. It results in synchronised tumbling and wobbling of the whole MNG accompanied by its volume oscillates. We show that the volume oscillations and rotations are two faces of the same periodic process whose frequency is a growing function of the shear rate and depends on strength of magnetic interaction between magnetic nanoparticles. We demonstrate that the oscillations of the volume lead to the periodic changes in MNG magnetic energy.