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VABILO NA PREDAVANJE
V OKVIRU DOKTORSKEGA ŠTUDIJA
KEMIJSKE ZNANOSTI

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z naslovom:

pH-dependent swelling and ionisation of weak polyelectrolyte and polyampholyte networks: A Monte Carlo study

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Vljudno vabljeni!

Abstract:

For weak polyelectrolytes (PE) as well as for weak polyampholytes (PA), not only the pH-pKA value but also the local electrostatic environment of the ionisable group determines the degree of ionisation and structural properties of the polymer. The proximity of already ionised groups, which is enforced by the interconnectivity of the polymer chain, influences the probability of additional groups to become ionised. Therefore, the degree of ionisation for polymers with different architectures differs from the ideal value, obtained for monomers at low concentrations. Linear PAs have been investigated theoretical [1] and in computer simulations [2]. PA with a network topology are interesting, because of their possible applications for the pH-triggered uptake and release of guest molecules.
In this work we investigate PE and PA networks with different distributions of the titratable groups within the network. We employ a bead-spring model of the polymers with ionisable beads, explicit counterions and implicit solvent. The model is solved using Monte Carlo simulations and we involve a special titration step, which includes both the intrinsic probability of ionisation for the isolated monomer as well as the interaction of the charge with its environment in the acceptance criterion of the trial move. We assess the degree of ionisation as well as the structure of the polymer in dependence of the pKA, pKB and pH values of the system for homopolymer polyelectrolyte networks as well as for amphoteric copolymers with different spatial distributions of acidic and basic monomers. Counterion distributions and the effective charge of the microgel were investigated as well.
It is seen, that for PE microgels, the degree of ionisation usually is reduced [3], whereas for polyampholyte microgels ionisation can either be reduced or enhanced depending on the type and distribution of the monomers of different type in network. In accordance with experiments, two titration steps are found for polyamphoteric polymer networks with relatively close pKA and pKB values. The degree of ionisation differs depending on the radial position of the titratable group within the microgel.

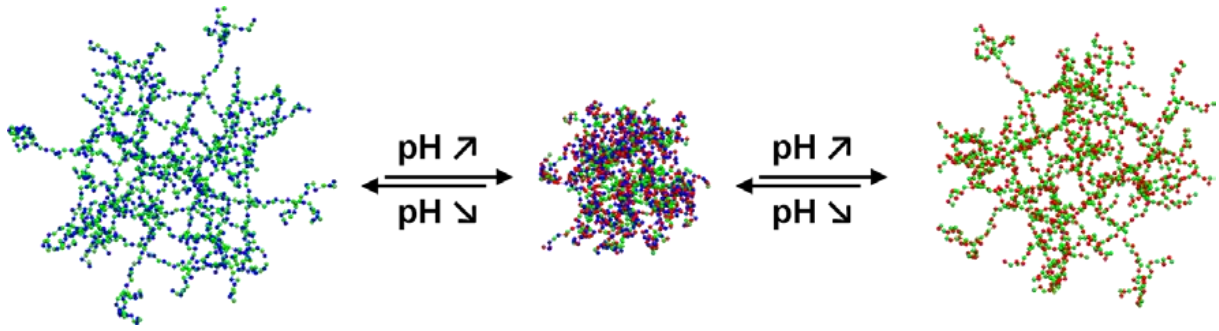

Figure 1. Snapshots of PA networks with a random distribution of acidic and basic groups at low (left), intermediate (center) and high (right) pH. Charged beads are depicted in blue (positive) and red (negative) and neutral beads are drawn in green color.

[1] A. Katchalsky, I. R. Miller, *J. Polym. Sci.,* 1954, ***13***, 57.
[2] S. Ulrich, M. Seijo, S. Stoll, *J. Phys. Chem. B,* 2007, ***111***, 8459.
[3] C. Hofzumahaus, P. Hebbeker, S. Schneider, Soft Matter, 2018, DOI: 10.1039/c7sm02528a