Inhomogeneous Structure of Swollen Microgels

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Microgels are cross-linked polymers, typically polyelectrolytes, with a network structure. They are able to undergo reversible volume phase-transitions in response to environmental stimuli such as pH, temperature, ionic strength of the surrounding medium, quality of solvent, and the action of the external electromagnetic field. This renders them potential candidates for a broad-range of applications in drug delivery, sensing, the fabrication of photonic crystals, template-based synthesis of inorganic nanoparticles, and separation and purification technologies. Microgels combine properties of dissolved macromolecules like the conformational flexibility and drainage by small molecules, with those of colloidal particles, like a defined shape and particle surface. The open structure allows for a compartmentalization inside the microgel with a swelling-induced tuneable porosity and controllable internal mobility of solvent and guest molecules, chain segments, as well as of the entire microgel. Therefore mass exchange with the surrounding is fundamentally different as compared to rigid colloidal particles.

To characterize their structural and dynamical properties, as well as the transport of small molecules in and out of a gelparticle, we perform large-scale computer simulation. We combine molecular dynamics simulations for the polymers and guest particles with the multiparticle collision dynamics approach for the solvent. Thereby, we perform simulations with and without hydrodynamic interactions. A microgel particle is comprised of a regular network of polymers connected by tetra-functional crosslinks. Each polymer is modeled as a self-avoiding chain composed of N_m monomers. In addition, electrostatic interactions are taken into account either by the Debye-Hückel potential (in a mean-field description) or by the Coulomb potential in the presence of counterions.

We present results for gelparticles of various sizes and polymer lengths. The influence of the charge-charge interaction strength is discussed on the microgel size, the radial monomer distribution, and, in case of explicit ions, the ion distribution inside and in the vicinity of the particle. Here, our studies provide a deep understanding on the detailed influence of a finite microgel size on its specific conformational properties.