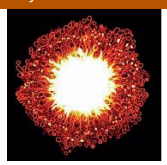

P.28 MD and COSMO-RS contact statistics for poly(N-isopropylacrylamide) in solvents

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The relatively new class of gels, the so-called microgels are chemically inert systems, which are responsive to changes of the environment by changing their shape and size. Therefore, an enormous potential in the area of drug delivery is attributed to microgels.

A phenomenon, which is not fully understood and still under debate in the literature, is the so-called cononsolvency effect. Thereby it can be observed that even if a particle is swollen in two pure solvents, it is collapsed in a mixture of the two solvents.

Molecular dynamics (MD) simulations were carried out to investigate the volume phase transition behaviour poly(N-isopropylacrylamide) (PNIPAM) polymer at the atomic level. Polymer chains consisting of 3 to 30 monomers units were solvated in water, methanol and water-methanol mixtures of different concentrations and/or different temperature below and above the lower critical solution temperature.

The COSMO-RS (Conductor-like Screening Model for Real Solvents) model allows for the predictive calculation of chemical potentials in almost arbitrary mixtures. It consists of a DFT (Density Functional Theory) calculation of each molecule in a virtual conductor, yielding the surface screening charge density distribution. Based on this, the interaction energies of molecules in contact are computed and thereby the chemical potential of each species are available. Therefore any thermodynamic data is available, including the phase transition behaviour.

As the surface contacts in the COSMO-RS model define all interaction properties, we analysed the MD trajectories for the purpose of molecular contact statistics by applying Voronoi tessellations to the configurations of the swollen and deswollen states of PNIPAM. The obtained results were compared with the COSMO-RS contact statistics. We expect that the analysing methodologies can be extended to other polymeric hydrogels and solvents, which will contribute to understand the observed phenomena and developing new polymer hydrogels with finely tuned characteristics.