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Co (non) solvency or the puzzle of polymer properties in mixed good or poor solvents

Kurt Kremer
Max Planck Institute for Polymer Research, Germany

The relation between atomistic structure, architecture, molecular weight and material properties is of basic concern of modern soft matter science. Here computer simulations on different levels of resolution play an increasingly important role. To progress further adaptive schemes are being developed, which allow for a free exchange of particles (atoms, molecules) between the different levels of resolution and thus pave the way to open systems simulations. Typical examples where such approaches are helpful are studies of stimuli responsive polymers, also called smart polymers. Here especially the so called co-solvency and co-non-solvency are puzzling examples of unusual polymer solvation behavior i.e. that of polymers in mixed solvents. Particularly PNIPAM in water alcohol mixtures reveals an interesting coil-globule-coil transition. This conformational transition cannot be explained within the classical Flory-Huggins picture, which is the standard mean field theory for polymer solutions and mixtures. The results point towards a general design of 'smart stimuli responsive polymers' and will be explored in detail. In the opposite case of a polymer in two poor solvents, e.g. PMMA in water and alcohol, a weak swelling is observed in mixed solvents. While appearing like just an inverse phenomenon of co-non-solvency, it turns out that here a delicate balance of depletion effects can be identified as the origin of the phenomenon.

kremer@mpip-mainz.mpg.de