The 2016 John D. Ferry Lectures in Physical Chemistry

Professor Kurt Kremer

Max Planck Institute for Polymer Research

Monday, February 15

2:00 pm, Room 1315 Chemistry

Reception to follow seminar in Shain Atrium

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

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. The extension to open systems MD (grand canonical MD) as well as recent Hamiltonian based molecular dynamics and Monte Carlo adaptive resolution methods will be explained. Typical examples include the solvation of polymers in mixed solvents, especially PNIPAM in water alcohol mixtures, which 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'. This work has been performed in collaboration with D. Mukherji and C. Marques.

Tuesday, February 16

11:00 am - Room 1315 Chemistry

Multiscale Simulations for Soft Matter: Applications and New Developments

The relation between atomistic structure, architecture, molecular weight and material properties is of basic concern of modern soft matter science. A typical additional focus is the relation between structure and function in nanoscopic molecular assemblies. Here computer simulations on different levels of resolution play an increasingly important role. This is achieved by two different approaches, namely by sequential multiscale descriptions or adaptive schemes, which allow for a free exchange of particles (atoms, molecules) between the different levels of resolution. The extension to open systems MD (grand canonical MD), as well as recent Hamiltonian based molecular dynamics and Monte Carlo adaptive resolution methods will be explained. A typical application for adaptive schemes is the solvation of polymers in mixed good solvents, called co(non)solvency, while structure formation of polymeric materials for organic electronics has been studied by a sequential scheme.