

SYLICA LECTURES:

You are cordially invited to the lectures delivered by

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WHERE: Meeting room, 4th floor, Faculty of Chemistry, Brno University of Technology, Purkyňova 118, Brno

Monday 19/05/2014, 9:30 a.m.: Slow Segmental Relaxation, Aging and Mechanical Response of Polymer Melts and Glasses

Slow dynamics in supercooled liquids and glasses is of widespread interest for diverse materials classes and scientific disciplines. The common physical feature is the critical importance of rare activated hopping motions which are very sensitive to temperature and external mechanical forces. A new statistical mechanical theory for the alpha relaxation process and shear modulus of equilibrium molecular and polymer liquids will be described that captures the rich experimental phenomenology over 14 decades in time as a consequence of a local activation event and its coupling to the emergent long range elasticity in cold liquids. The approach has been extended to the quenched nonequilibrium polymer glass state based on the experimentally-measurable amplitude of nanometer scale density fluctuations as the central collective variable. Building on this advance, a theory for physical aging and mechanical response under both constant stress (creep) and constant strain rate conditions has been constructed. The nonlinear competition between the effects of aging and mechanical rejuvenation on density fluctuations, relaxation, and mechanical properties will be discussed, and quantitative applications to PMMA glasses presented.

Tuesday 20/05/2014, 9:30 a.m.: Structure, Diffusion and Entanglement Phenomena in Polymer Nanocomposites

Polymer nanocomposites are hybrid mixtures of hard nanoparticles and soft macromolecules that display novel and diverse microstructures, properties, and dynamical phenomena even in the molten state. We have developed a microscopic theory for the equilibrium structure and phase behavior of such systems that provides guidelines for realizing three qualitatively different spatial organizations of nanoparticles. Quantitative comparisons to x-ray and neutron scattering experiments on silica-based materials will be presented. We have also developed a dynamical theory for nanoparticle transport in unentangled and entangled polymer liquids that accounts for multiple non-hydrodynamic effects and failure of the Stokes-Einstein relation. Its predictions for diffusivity under dilute filler loading conditions are in very good agreement with recent computer simulations and experiments. At higher nanoparticle concentrations, polymer dynamics is modified in a length-scale-dependent manner. I will discuss a first principles theory of such effects for rigid rod and flexible chain polymer nanocomposites, focusing on how the modification of topological entanglements impacts the tube diameter and macromolecule anisotropic diffusivity.

