



Department of Chemistry

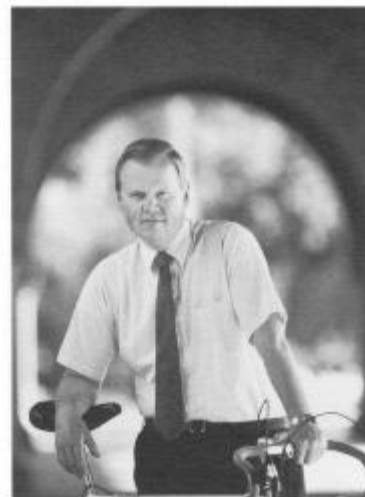
Presents

Dr. Hans C. Andersen

Professor, Department of Chemistry
Stanford University

Wednesday, Sept 24, 2008
Dell Butcher Hall 180 - 2:30 p.m.

Refreshments served at Seminar



***“Scaling Analysis of Dynamic Heterogeneity
in a Supercooled Lennard-Jones Liquid”***

Dynamic heterogeneity has been recognized as a significant feature of supercooled liquids. At any given time, there are some regions of such a material in which the molecules are more mobile and hence relaxation takes place at rates that are larger than the average relaxation rates in the material. Moreover, the correlation length that characterizes the sizes of these regions increases as the temperature is lowered. This behavior has been observed in computer simulations and inferred from experimental measurements on several kinds of materials. We have performed molecular dynamics computer simulations of a dense Lennard-Jones liquid mixture to study dynamic heterogeneity from normal liquid temperatures down to a supercooled temperature 15% above the previously identified mode coupling temperature T_c of the model. A susceptibility associated with the correlation function of mobility fluctuations was defined and calculated from simulation data as a function of wave vector and temperature. A correlation length for mobility fluctuations was obtained from the wave vector dependence for each temperature. The results were used to test two sets of scaling hypotheses for the liquid. The first set is based on the idea that the mobility correlation function obeys a scaling principle in which the only relevant length scale is the correlation length. The second set of hypotheses is based on the temperature dependence of singular functions predicted by mode coupling theory. The results are in close agreement with the inhomogeneous mode coupling theory of Biroli *et al.* [Phys. Rev. Lett. 97, 195701 (2006)] for both the α and β relaxation regimes. Comparison with results for kinetically constrained models suggest that the Lennard-Jones mixture studied is more similar to models for fragile liquids than models for strong liquids.

About the Speaker

Dr. Hans C Andersen, Professor, Department of Chemistry, Stanford University received his B.S. and Ph.D. from the Massachusetts Institute of Technology. Awards: Sloan Foundation Fellow, 1972-74; John Simon Guggenheim Fellowship, 1976-77; Hildebrand Award of the American Chemical Society, 1988; Member, National Academy of Sciences, 1992; Dean's Award for Distinguished Teaching, Stanford, 1992; Theoretical Chemistry Award, American Chemical Society, 2006

Host: Dr. Gus Scuseria, Robert A. Welch Professor; Department Vice Chair