



Concordia
UNIVERSITY



**Joint Seminar Series of the
CENTRE FOR RESEARCH IN MOLECULAR MODELING
and the
DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY**

April 26, 2002, 2:15 pm - Concordia University H-1070

Effects of (Micro)heterogeneities on Solvation Dynamics

Prof. Branka M. Ladanyi

Department of Chemistry, Colorado State University

Solvation dynamics is the rate of solvent reorganization in response to a change in solute-solvent interactions. It is usually measured by monitoring the time-evolution in the solvatochromic shift in the fluorescence spectrum of a dissolved dye molecule. We use theory and molecular dynamics computer simulation to investigate the solvation dynamics mechanisms in a variety of fluid environments. This talk will address how structural and dynamical heterogeneities in confined liquids and preferential solvation in dipolar-quadrupolar mixtures affect the dynamic response of the solvent to electronic excitation which changes the charge distribution of a dissolved chromophore. In the first case, we investigate solvation dynamics in the aqueous phase of water-in-oil microemulsions using a model that we have recently developed for the water pool of reverse micelles formed by the anionic surfactant Aerosol-OT. In the second case, we investigate the solvation mechanisms contributing to the composition-dependence of solvation dynamics in benzene-acetonitrile mixtures. For solvation dynamics in reverse micelles we study the effects of the size of the water pool and the location of the chromophore within it, of the restricted water mobility and of the presence of sulfonate head groups and Na^+ counterions. For benzene-acetonitrile mixtures we find that a solute resembling the coumarin 153 chromophore is preferentially solvated by acetonitrile in the excited, but not in the ground electronic state. We investigate how the build-up of the local concentration enhancement contributes to the mechanism and time scale of solvation dynamics of mixtures of different composition. If time allows, the effects of local density augmentation on solvation dynamics in supercritical fluids will also be discussed.

Branka M. Ladanyi graduated in 1969 from McGill University with First Class Honours in Physics and was awarded the Horace Watson Gold Medal. She then went south of the border to the United States to pursue graduate study in physical chemistry at Yale University, where she earned a Ph.D. in 1973. After postdoctoral studies at the University of Illinois and Yale University, she joined the Chemistry Department at Colorado State University as an Assistant Professor in 1979 and was promoted to Professor in 1987. Dr. Ladanyi was awarded the Alfred P. Sloan Fellowship in 1982 and became a Camille and Henry Dreyfus Teacher-Scholar in 1983. She was a Visiting Fellow at the Joint Institute for Laboratory Astrophysics in 1993-94. She was elected to Fellowship in the American Physical Society in 1997. Dr. Ladanyi's professional service has included work on review and advisory panels for scientific granting agencies within the United States and internationally, including for the US National Science Foundation and Department of Energy and for the Swedish National Science Foundation. She was a member of the editorial advisory board for the Journal of Molecular Liquids 1993-99 and has been an Associate Editor of the Journal of Chemical Physics since 1994. Her research has focused mainly on the theory of liquid state systems. It has produced over a hundred of research articles published in major peer-reviewed journals as well as several review articles and book chapters. She has trained a number of scientists who have gone on to successful careers in academia, industry and government laboratories in North and South America, Europe, and Asia.

