

of the breakdown of the Stokes-Einstein relation that has been observed in many glass forming liquid systems near the glass transition temperature. We have also studied implications of the dynamical heterogeneities on recent single molecule experiments of glass forming liquids. We investigate the distribution of the dynamical heterogeneities probed by single probe molecules over different coarse-graining timescales through numerical simulations. Based on our simulation results, we propose a new experimental measurement involving correlations among single probe molecules that will provide information on the distributions of dynamical heterogeneity.

**78. SELF-DIFFUSION NEAR TG IN SINGLE COMPONENT GLASS FORMERS.** *Mark D. Ediger, and Stephen Swallen, Department of Chemistry, University of Wisconsin, 1101 University Avenue, Madison, WI 53706, Fax: 608-262-0381, ediger@chem.wisc.edu*

The self-diffusion coefficient is arguably the single most important measure of mobility in a liquid. We present the first direct measurement of self-diffusion of a single-component glass-forming liquid at the glass transition temperature. Forward Recoil Spectrometry (FRoS) is used to measure the concentration profiles of deuterio and protio 1,3-bis-(1-naphthyl)-5-(2-naphthyl)benzene (TNB) following annealing-induced diffusion in a vapor deposited bilayer. These experiments extend the range of measured diffusion coefficients in TNB by 6 orders of magnitude. While rotational correlation times have previously been found to track the viscosity, these new results indicate a decoupling of translational diffusion from viscosity or rotation. At  $T_g$ ,  $D$  is 500 times larger than expected from the Stokes-Einstein equation. These results are qualitatively consistent with previous measurements of dye diffusion in TNB and explain the unusual temperature dependence of crystal growth rates in TNB.

**79. SINGLE-PARTICLE DYNAMICS IN DEEPLY SUPERCOOLED LIQUIDS.** *John T. Fourkas<sup>1</sup>, Thomas J. Kempa<sup>2</sup>, Richard A. Farrer<sup>2</sup>, and Robert M. Dickson<sup>3</sup>. (1) Department of Chemistry, Boston College, Merkert Chemistry Center, 2609 Beacon St., Chestnut Hill, MA 02467, Fax: 617-552-6887, fourkas@bc.edu, (2) Eugene F. Merkert Chemistry Center, Boston College, (3) School of Chemistry and Biochemistry, Georgia Institute of Technology*

Photoluminescence from metallic nanoparticles with nanometer diameters has been used to study orientational dynamics in a deeply supercooled liquid, 4,4'-(octahydro-4,7-methano-5H-inden-5-ylidene) bisphenol dimethyl ether (ODE). We explore the dependence of the bulk orientational correlation time on the bulk ODE viscosity to show that nanoparticles can provide a useful probe of local dynamics, and we discuss single-particle orientational diffusion trajectories. We will also compare the information available from two- and three-dimensional orientational trajectories.

**80. QUENCHING-IN OF DIFFERENT HIGH T COMPLEXITIES OF GLASSFORMERS FOR LEISURELY STUDY AT LOWER TEMPERATURES.** *C. Austen Angell<sup>1</sup>, Yuanzheng Yue<sup>2</sup>, Li-Min Wang<sup>1</sup>, John R. D. Copley<sup>3</sup>, Steve Borick<sup>4</sup>, and Stefano Mossa<sup>5</sup>. (1) Department of Chemistry and Biochemistry, Arizona State University, Main Campus, P.O. Box 871604, Tempe, AZ 85287, Fax: 480-965-7972, caa@asu.edu, (2) Chemistry, University of Aalborg, (3) National Institute of Standards, (4) Scottsdale Community College, (5) Center for Statistical Mechanics and Complexity, Università di Roma*

We describe a series of experiments on glass-forming liquids that are motivated by a common idea. The idea is that of trapping in a high enthalpy, high entropy, state of the system by quenching to the glassy state at extreme rates, and then observing the way the system evolves at low temperatures during a controlled

annealing procedure. In this manner, events that normally occur during change of temperature may be observed occurring during passage of time, at much lower temperatures. At these low temperatures, the smearing effects of vibrationally excited modes may be greatly reduced. For simple glassformers we study both relaxational properties and vibrational properties and find that the high fictive temperature states are characterized by short relaxation times (already known) and considerably more intense boson peaks (less well known). The thermodynamic consequences of the increased populations of these low frequency modes are examined with the help of computer simulation and normal mode calculations on model glassformers. Behavior in the vibrational DOS at constant pressure is strikingly different from that at constant volume. For glassformers that can exhibit liquid-liquid transitions, one can use the cold equilibration approach to determine the fragility of the high temperature phase, and the enthalpy of the liquid-liquid transition. Finally, for solutions of complex molecules with interesting internal molecular transitions, such as proteins, we can quench in the unfolded states and then, using special non-crystallizing solvents, observe the molecular reorganization to low energy states as it occurs at temperatures far below the normal folding temperature.

**81. ANATOMY OF A STRING: CORRELATED PARTICLE MOTION IN SIMULATED SUPERCOOLED LIQUIDS.** *Sharon C. Glotzer, Yeshitila Gebremichael, Michael Vogel, and Magnus Bergröth, Department of Chemical Engineering, University of Michigan, Ann Arbor, MI 48109, sglotzer@umich.edu*

We present new results of a detailed investigation of correlated particle motion in model supercooled liquids studied via molecular dynamics simulation. We investigate in particular the tendency for correlated motion to occur in strings. We present a detailed analysis that elucidates how and why strings form, the degree of coherence of particle motion within strings, the lifetime of strings, and the role of strings in facilitating structural relaxation in the liquid.

**82. EVOLUTIONARY PERSPECTIVES ON PROTEIN FOLDING, STRUCTURE, AND THERMODYNAMICS.** *Richard A. Goldstein, Department of Chemistry, University of Michigan, Ann Arbor, MI 48109-1055, Fax: 734-647-4865, richardg@umich.edu*

Proteins fold into their native-state conformations in milliseconds to seconds, ignoring theoretical estimates that this process should take many times the age of the universe. Much work is directed to understanding how proteins are so much smarter than theorists, who cannot even reliably predict what the final folded states will be. Proteins have one major advantage over theorists - proteins have been working on this problem for billions of years. We can consider different ways in which proteins may have evolved to solve the protein-folding problem. Using simple theoretical models, we can show how neutral evolution and population dynamics combined with the need to fold can explain many of the observed properties of proteins, including the way proteins fold, the distribution of observed protein structures, the marginal stability of proteins, and how the evolutionary robustness of protein structures co-exists with sequence plasticity.

**83. PROTEIN BUILDING BLOCKS FOR RECOMBINATION.** *Zhen-Gang Wang, Division of Chemistry and Chemical Engineering, California Institute of Technology, 1200 E. California Blvd., Mail Code 210-41, Pasadena, CA 91125, Fax: 626-568-8743, zgw@cheme.caltech.edu*

In vitro recombination is a powerful tool for tuning and optimizing protein functions. It promotes the rapid accumulation of beneficial traits from multiple