Invited Lecture
Inter-Disciplinary Explorations in Chemistry (I-DEC 2018)

Dielectric Relaxation in Acetamide+Urea Deep Eutectics: Possible Origin of the Multi-Step Relaxations

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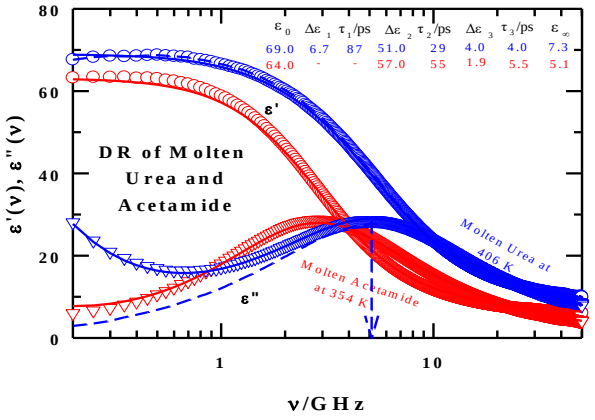
Dielectric relaxation (DR) measurements in the MHz-GHz regime for deep eutectic solvents (DESs) made of acetamide (CH_3CONH_2) and urea (NH_2CONH_2) reveal three distinct relaxation timescales.[1] Similar multi-step relaxations have been observed in the DR of neat molten urea. The slowest of multi-step DR relaxation times (τ_1) resembles closely to the longtime constant of the simulated structural H-bond relaxation ($C_{HB}(t)$) involving urea pairs. Similarity, activation energies estimated from the temperature dependent DR measurements ($335 \leq T/K \leq 363$) and structural H-bond relaxations indicates that the structural H-bond relaxation overwhelmingly dominates the slowest DR relaxation in these DESs. Simulated collective reorientational correlation functions ($C_\ell(t)$), on the other hand, suggest that collective the single particle orientation dynamics also contribute, albeit partially, to the observed total relaxation. Fractional viscosity dependence for the longest DR times, $\tau_{DR} \propto (\eta/T)^p$, has been observed for these DESs. Simulated four point correlation functions qualitatively explain, via the estimated correlated length- and time-scales, the origin of this fractional viscosity dependence. In addition, these estimated dynamical time- and length-scales assist in understanding the different inferences regarding solution heterogeneity drawn from different measurements on these DESs.

Reference: 1. K. Mukherjee, S. Das, E. Tarif, A. Barman, and R. Biswas, *J. Chem. Phys.* **2018**, *149*, 124501/1-12.



Bio-Sketch of Speaker

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Ranjit Biswas, after acquiring BSc. (Chemistry Honours) and MSc (Inorganic special) degrees from the Kalyani University, West Bengal, obtained his PhD degree in Theoretical Physical Chemistry after working with Professor Biman Bagchi in the Indian Institute of Science, Bangalore during 1993-1998. He then proceeded for his post doctoral research in experiments in the laboratory of Professor Mark Maroncelli, Pennsylvania State University, USA where he stayed four years (1998-2002) to learn and use ultrafast fluorescence measurement methods for measuring relaxation dynamics in condensed phases. After joining the S. N. Bose National Centre for Basic Sciences (SNBNCBS), Kolkata in 2002, he established spectroscopy laboratories and computational facilities (both as central equipments/facilities) for performing research integrating experiments, theory and computer simulations. Currently Ranjit Biswas is serving as a Senior Professor. Eleven students have received PhD from his research group so far, five of whom are already absorbed in various universities and IITs as faculty members. At present ten students are working in his group for PhD. Ranjit Biswas has also been involved in several high value institutional projects as one of the Principal Investigators, one of them being the Technology Research Centre (TRC) in the SNBNCBS. A part of his time is now dedicated to translate relevant basic scientific knowledge into development of analyses tool that can impact a significant section of the society.