Ranjit Biswas

Professor
CBMS
ranjit@bose.res.in

In the research group of Prof. Ranjit Biswas, they perform experiments, develop theory and employ computer simulations to generate an integrated understanding of chemical events in complex systems. Their research has led to significant insights into the (i) structure and dynamics of deep eutectic solvents, (ii) relaxation mechanism in ionic liquids and (ionic liquid + polar solvent) binary mixtures, (iii) aggregation in aqueous solutions (iv) slow dynamics in confined aqueous environments and (v) mechanism that decouples solute rotation from electrostatic interactions.

Supervision of Research / Students

Ph.D. Students

1. Kajal Kumbhakar, Experiments, Chemical Dynamics in Complex Systems, Ongoing.
2. Atanu Bakshi, Theoretical Studies of Relaxation Dynamics in Confinements and Ionic Systems, Theory & Simulations, Ongoing
3. Juriti Rajbangshi, Studies of Glassy Signatures in High Temperature Systems, Simulations, Ongoing
4. Ejaj Tarif, Experiments Relaxation Dynamics in Complex Chemical Systems, Ongoing.

Teaching activities at the Centre

1. CB524 Physical Chemistry: Experiments & Theory

Publications in Journals

1. S. Rajkhowa, S. Mahiuddin, J. Dey, S. Kumar, V. K. Aswal, **R. Biswas,** J. Kohlbrechere and K. Ismail; *The Effect of Temperature, Composition and Alcohols on the Microstructures of Catanionic Mixtures of Sodium Dodecylsulfate and Cetyltrimethylammonium Bromide in Water;* Soft Matter; 2017; **13;** 3556-3567; DOI: 10.1039/c7sm00342k.
2. Kallol Mukherjee, Ejaj Tarif, Anjan Barman and **Ranjit Biswas;** *Dynamics of a PEG Based Non-Ionic Deep Eutectic Solvent: Temperature Dependence;* Fluid Phase Equilibria; 2017; **448;** 22-29; Invited Article for the Special Issue on Deep Eutectic Solvents; DOI: 10.1016/j.fluid.2017.05.003.
3. Suman, Das, Biswaroop Mukherjee and **Ranjit Biswas;** *Microstructures and Their Lifetimes in Acetamide/Electrolyte Deep Eutectics: Anion Dependence;* Journal of Chemical Sciences; 2017; **129** (7); 939-951; Invited Article for Charusita Chakrabarti special issue; DOI: 10.1007/s12039-017-1263-9.
4. Sandipa Indra and **Ranjit Biswas;** *How Heterogeneous Are Trehalose/Glycerol Cryoprotectant Mixtures? A Combined Time-Resolved Fluorescence and Computer Simulation Investigation;* Journal of Physical Chemistry B; 2016; **120;** 11214-11228.
5. Sandipa Indra and **Ranjit Biswas;** *Is Dynamic Heterogeneity of Water in Presence of a Protein Denaturing Agent Different from that in Presence of a Protein Stabilizer? A Molecular Dynamics Simulation Study;* Journal of Chemical Sciences; 2016; **128;** 1943-1954.
6. Suman Das, **Ranjit Biswas** and Biswaroop Mukherjee; *Collective Dynamic Dipole Moment and Orientation Fluctuations, Cooperative Hydrogen Bond Relaxations, and Their Connections to Dielectric Relaxation in Ionic Acetamide Deep Eutectics: Microscopic Insight from Simulations;* Journal of Chemical Physics; 2016; **145;** 084504.
7. Kallol Mukherjee, Anjan Barman and **Ranjit Biswas;** *Impact of the Aggregation Behaviour of Sodium Cholate and Sodium Deoxycholate on Aqueous Solution Structure and Dynamics: A Combined Time Resolved Fluorescence and Dielectric Relaxation Spectroscopic Study;* Journal of Molecular Liquids – Special Issue (Invited Article); 2016; **222;** 495-502.

Lectures Delivered

1. Invited Talk in the Indo-Japan Meeting, Department of Chemistry, IIT-Kanpur on November 15, 2016, entitled 'Dielectric Relaxation in Ionic and Non-Ionic Deep Euetctics: Polarity and Origin of Relaxation Timescales'.

Membership of Committees

Internal Committee

HoD/CBMS; Convener, SCOLP-EVLP

Collaborations including publications (Sl. No. of paper/s listed in 'Publications in Journals' jointly published with collaborators)

National

1. Sl. No. 1

International

1. Sl. No. 1

Significant research output / development during last one year

General research areas and problems worked on

- Structure & Dynamics of Deep Eutectics
- Understanding glass dynamics of coulomb systems/ fluids
- Small molecule relaxation in a wide variety of environments

Interesting results obtained

The research works of R. Biswas and his students/ collaborators are concerned with the central theme of developing a molecular level understanding of the structure and dynamics of complex media and their relationship to simple chemical events occurring in them. For this, Dr. Biswas performs experiments, and carries out computer simulations and theoretical studies in his own group. This approach constitutes a rather interesting example where results obtained by one method are analyzed and complemented with the data provided by the other two.

The above trend is reflected in various research papers published by Biswas et al in the last few years. For example, the first molecular theory for experimental Stokes shift dynamics in ionic liquids (ILs) emerged from this research group. These works have successfully explained the experimental results obtained via ultrafast fluorescence measurements of ILs. Temperature-dependent studies have explained why hydrodynamics nearly holds for diffusive relaxations in these highly viscous and heterogeneous media. The prediction 4 that the motion of a large solute can influence the relaxation in these Coulomb fluids has been validated by subsequent simulation works. Further study reveals a strong interconnection between the measured sub-picosecond fluorescence response in ILs and rotation of dipolar ions in a collective potential created by the ionic neighbors.

The first semi-molecular theory for understanding experimental Stokes shift dynamics in (IL + common polar solvent) mixtures has also originated from this research group. An extremely slow (just a few nanoseconds) time-scale in the collective orientational relaxation appears in an all-atom simulation study of (ionic liquid + real solute). These works constitute a fundamental contribution to the overall understanding of relaxation processes in ILs.

Interaction and dynamics in deep eutectic solvents have been explored by using fluorescence experiments, simulations and theory by this group. These studies are novel in the sense that these works for the first time focused on the chemical physics of deep eutectics. These mixtures resemble ionic liquids (interaction-wise) yet show diffusion-viscosity decoupling at a much higher temperature. A combined fluorescence and all-atom simulation study provides emphatic evidences for the existence of ultra-slow water in confined aqueous systems, and explains numerous experimental results including theirs. Picosecond fluorescence dynamics studies of (alcohol + water) binary mixtures are well-cited works as these have made important contributions in understanding the hydrophobic interaction induced water agglomeration in aqueous solutions. In a very recent work, the first evidence for electrolyte-induced arrest of polymer segmental motion in polymer-electrolyte composites has been observed. Other simulation studies and analytical works depict microscopic picture of interaction and dynamics in liquid mixtures, electrolyte solutions and super-critical fluids.

Very recently, presence of jump reorientations in molten acetamide has been established, and extended to ionic acetamide deep eutectics. High frequency response in ionic and non-ionic deep eutectics has been measured and their impact on a chemical reaction studied. Experimental study exploring competition between hydrophobic interaction and critical fluctuations in producing microheterogeneity in binary mixtures with solubility gap has been performed and heterogeneity length- and timescales in binary mixtures explored. Furthermore, aggregation behavior of a variety of molecules has been studied and impact on dynamics explained via carrying out simulations and measurements. In summary, these works are of a high quality and have provided a critical understanding of several longstanding fundamental questions in solution-phase physical chemistry.

Proposed research activities for the coming year

Generating better understanding of deep eutectic solvents.