Ranjit Biswas
Senior Professor
CBMS
ranjit@bose.res.in

Guidance of Students/Post-Docs/Scientists

a) Ph.D. Students

1. Juriti Rajbangshi; Computer Simulations of Complex Chemical Systems; Thesis submitted
2. Ejaj Tarif; Experimental studies of deep eutectics; Awarded
3. Kajal Kumbhakar; Experimental Studies of Energy Materials; Awarded
4. Atanu Baksi; Computer Simulations of Aqueous & Other Systems; Thesis submitted
5. Narayan Maity; Experimental Studies of Metastable and Self-Organised Systems; Under progress
6. Jayanta Mondal; Experimental Studies of Ionic and Neutral Deep Eutectics; Under progress
7. Dhrubajyoti Maji; Computer Simulations of Deep Eutectics; Under progress
8. Amrita Mondal; Experimental Studies of Complex Chemical Systems; Under progress
9. Sudipta Mitra; Computer Simulations of Relaxation Dynamics in Condensed Phases; Under progress
10. Rik N Mukherjee; Computer Simulations of Ionic Deep Eutectic and Other Systems; Under progress

Publications

a) In journals

1. Swarup Banerjee, Pradip Kr. Ghorai, Suman Das, Juriti Rajbangshi, and **Ranjit Biswas**, *Heterogeneous dynamics, correlated time and length scales in ionic deep eutectics: Anion and temperature dependence*, The Journal of Chemical Physics, 153, 234502, 2020
2. Atanu Baksi and **Ranjit Biswas**, *Does Confinement Modify Preferential Solvation and H-Bond Fluctuation Dynamics? A Molecular Level Investigation through Simulations of a Bulk and Confined Three-Component Mixture*, The Journal of Physical Chemistry B, 124, 11718 – 11729, 2020
3. Juriti Rajbangshi, Swarup Banerjee, Pradip Kr. Ghorai and **Ranjit Biswas**, *Cosolvent polarity dependence of solution structure in [BMIM] [PF$_6$] + acetonitrile/1, 4-dioxane/hexane binary mixtures: Insights from composition dependent Voronoi polyhedra analyses, iso-surfaces and radial distribution functions*, Journal of Molecular Liquids, 317, 113746, 2020
4. Atanu Baksi, Pradip Kr. Ghorai, and **Ranjit Biswas**, *Dynamic Susceptibility and Structural Heterogeneity of Large Reverse Micellar Water: An Examination of the Core–Shell Model via Probing the Layer-wise Features*, The Journal of Physical Chemistry B, 124, 2848-2863, 2020

Areas of Research

Physical Chemistry Chemical Physics, Experiments (Spectroscopy), Theory & Simulations

Exploring the local environment around a dissolved solute in a bulk aqueous solution of alcohol and assessing the impact of confinement on the solvation structure is an important topic yet much less studied. Such a study is important because it can provide critical information regarding the miscibility of an amphiphilic drug after delivery at a designated nanoscopic site and the subsequent release. The present molecular dynamics simulation study reports an in-depth investigation of the composition-dependent solvation structure around a dissolved hydrophobic solute, coumarin 153 (C153), in ambient binary mixtures of methanol and water in both bulk and under confinement. The confinement is a spherical sodium bis(2-ethylhexyl) sulfosuccinate (AOT) reverse micelle with a diameter of 55 Å. Inter- and intraspecies H-bond fluctuation dynamics have been monitored and compared with those from the corresponding bulk binary mixtures. It has been observed that confinement accentuates the preferential solvation phenomenon and facilitates the di-mixing of mixture components. The present study reveals that the tetrahedral H-bond network of neat liquid water becomes severely affected upon the addition of methanol, which becomes further distorted under confinement. Interestingly, structural hydrogen bond relaxation timescales become longer in confined binary mixtures than in bulk binary mixtures.

Heterogeneous relaxation dynamics often characterizes deep eutectic solvents. Extensive and molecular dynamics simulations have been carried out in the temperature range, $303 \leq T/K \leq 370$, for studying the anion and temperature dependencies of heterogeneous dynamics of three different ionic acetamide deep eutectics: acetamide + LiX, X being bromide (Br−), nitrate (NO − 3), and perchlorate (ClO − 4). These systems are chosen because the fractional viscosity dependence of average relaxation rates reported by various measurements has been attributed to the heterogeneous dynamics of these systems. Simulations performed here attempt to characterize the heterogeneous relaxation dynamics in terms of correlated time and length scales and understand the solution inhomogeneity in microscopic terms. Additionally, simulation studies for pure molten acetamide have been performed to understand the impact of ions on motional features of acetamide in these ionic deep eutectic systems. The computed radial distribution functions suggest microheterogeneous solution structure and dependence upon anion identity and temperature. A significant plateau in the simulated time dependent mean squared displacements indicates pronounced cage-rattling and inhomogeneity in relaxation dynamics. Simulated diffusion coefficients for acetamide and ions show decoupling from the simulated viscosities of these deep eutectics. Calculated two- and four-point correlation functions reveal the presence of dynamic heterogeneity even at 180 K above the measured thermodynamic glass transition temperature (Tg). Further analyses reveal the existence of multiple timescales that respond strongly to the rise in solution temperature. The simulated dynamic structure factor and overlap function relaxations show strong stretched exponential relaxations. The simulation results support the experimental observation that the bromide system is the most dynamically heterogeneous among these three systems. Correlated length scales show much weaker anion and temperature dependencies with an estimated length of 1 nm, suggesting formation of clusters at the local level as the origin for the micro-heterogeneous nature of these ionic deep eutectics.