Index No.: 31/19/Chem./26

Abstract

The thesis entitled "**Understanding the Structural and Dynamical Complexities of Neat and Multi-component Media**" investigates the structure and relaxation dynamics of various neat solvents and multi-component complex media. By delving into the fundamental aspects of these systems, this research aims to enhance our understanding of their behaviour and properties, contributing to the advancements in fields such as pharmaceuticals, cryopreservation, energy storage, and biomedical applications. The goal is to provide a foundation for further research and practical applications where fundamental scientific understanding is lacking.

The first begins with the investigating water-octanol mixtures across various water mole fractions, which are pivotal in structural biology, drug delivery, and pharmaceutical chemistry. The second focus is to explore the interaction, dynamics, and solution heterogeneity in multi-component cryoprotectant mixtures with glucose/ethylene glycol and disaccharides dehydrates/glycerol based cryoprotectant mixtures (where disaccharides used as trehalose and sucrose) which are biodegradable, non-toxic and cheap cost, and play a crucial role in preserving organ, live cell, tissues, DNA, proteins and other substances at very low temperatures. The third area of interest is to explore the interaction and dynamics of electrolyte media used in lithium-ion batteries, capacitors, and energy storage devices for electrical vehicles. The fourth area of interest is the investigation of the sol→gel transition of biopolymer in aqueous media, which undergo structural transitions in response to external stimuli such as agitation or temperature. Understanding the structure, interaction, and relaxation dynamics of this biopolymer is essential for the development of tissue engineering, cell culture, and bioscaffold, particularly in the biomedical field of fibrosis leading to organ dysfunction.

In this thesis, dielectric relaxation (DR) spectroscopy is employed in the Hz-GHz frequency range (20 HZ to 50 GHZ) to investigate the reorientation dynamics of dipolar species in specific media. To elucidate system interactions and spatial-temporal heterogeneity, the research employs steady-state fluorescence, and time-resolved fluorescence (TRF) techniques, including time-correlated single photon counting (TCSPC) and two-dimensional streak camera (2DSC) measurements. Additionally, a variety of experimental techniques and computer simulations are employed to thoroughly investigate these complex media. Such experiments are dynamic light scattering (DLS), differential scanning calorimetry (DSC), and cryo-transmission electron microscopy (cryo-TEM).

Narayan Chandra Maity
20.08.24

Ranjit Biswas
20.08.24

DR. RANJIT BISWAS
Senior Professor
Dept. of Chemical, Biological & Macromolecular Sciences
S. N. Bose National Centre for Basic Sciences
Block - JD, Sector-III, Salt Lake, Kolkata - 700 106, India

Chapter 1 of this Thesis provides an introductory overview of the research work and reviews pertinent literature. In Chapter 2, a succinct explanation of the experimental techniques and data analysis procedures employed in this Thesis is presented. Moving on to Chapter 3, a thorough investigation is undertaken on octanol-water mixtures within the octanol-rich region. This exploration unveils water concentration-dependent alterations in structure, reorientation dynamics, intra and inter-species hydrogen bonding, and dielectric properties of these mixtures, along with variations in angle distribution and tetrahedral order parameters of water. This comprehensive analysis is conducted through experimental techniques such as DRS and DSC, coupled with computer simulations. Chapter 4 provides an exploration of the interactions, dynamics, and solution heterogeneity of pure octanol and water/octanol mixtures. This investigation employs steady state fluorescence and TRF measurements within the temperature range of $283 \leq T/K \leq 323$, considering various mole fractions of water in the octanol-rich aqueous solution. In Chapter 5 and Chapter 6, an extensive investigation is conducted on glucose concentrations dependent glucose/ethylene glycol cryoprotectant mixtures, exploring various aspects such as thermo-physical properties, particle size, reorientation relaxation dynamics, ultrafast Stokes dynamics, viscosity coupling, and solution heterogeneity. This comprehensive exploration utilizes diverse experimental techniques, including DSC, DLS, DRS, steady state fluorescence, TRF-2DSC, and TRF-TCSPC measurements. In Chapter 7, a systematic investigation unfolds, delving into the interaction, dynamics, and solution structure of disaccharides dihydrate/glycerol cryoprotectant mixtures. This exploration employs a combination of experimental techniques and molecular dynamics simulation methods. Chapter 8, a detailed exploration of the co-solvent concentration-dependent melting temperature, conductivity, dielectric properties, reorientation relaxation dynamics, and viscosity coupling of LIB electrolytes are explored through experiments. Additionally, molecular-level insights into solvation structure, component-wise diffusion, transport number, and ionic conductivity are revealed through molecular dynamics simulations. Chapter 9 focuses on the investigation of sol→gel transition with hyaluronic acid (HA) concentration (wt% of HA= 0, 0.15, 0.3, 0.5, 0.65, 0.75, 1, 1.5, 2). This exploration is carried out through refractive index measurement and steady-state fluorescence intensity measurement of Triflavin-T (ThT). The chapter also explores the hydrogel structure, reversibility, and the interactions of different organic fluorophore solutes to gain insights into the characteristics of hydrogels that could find applications in various fields and address pathology and dysfunction health issues in humans. Finally, Chapter 10 wraps up the thesis by providing concluding remarks and highlighting important areas for future exploration.

Narayan Chandra Maity
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DR. RANJIT BISWAS
Senior Professor
Dept. of Chemical, Biological & Macromolecular Sciences
S. N. Bose National Centre for Basic Sciences
JD, Sector-III, Salt Lake, Kolkata - 700 106, India