Rajib Kumar Mitra

Professor
CBMS
rajib@bose.res.in

Guidance of Students/Post-Docs/Scientists

a) Ph.D. Students

1. Sk. Imadul Islam; Studies on ultrafast dynamics and spectroscopic investigations on fluorescent probes in bimolecular and biomimetic recognition; Under progress
2. Saikat Pal; Studies on the Effects of Different Crowding agents on Protein FoldingUnfolding Process and its Kinetics as well as Activity; Under progress
3. Partha Pyne; Studies of Some Biophysical Processes Using Ultrafast Spectroscopic Techniques; Under progress
4. Anulekha De; Nanomagnetism; Thesis submitted; Prof. Anjan Barman (Co-supervisor)
5. Didhiti Bhattacharya; Opto-electronic, Electrical and Spectroscopic studies of two dimensional materials; Under progress; Prof. Samit K. Ray (Co-supervisor)
6. Sumana Pyne; Application of Ultrafast Spectroscopy in Biological Systems; Under progress
7. Sudip Majumder; Nanomagnetism; Under progress; Prof. Anjan Barman (Co-supervisor)
8. ia Saha; Studies on the Effects of Different Crowding agents on Protein Folding Unfolding Process and its Kinetics as well as Activity; Under progress
9. Subhajit Singha; Application of Ultrafast Spectroscopy in Chemical/Biological Systems; Under progress

b) Post-Docs

1. Bibhab Bandhu Majumdar; Protein folding under stressed environments

Teaching

1. Autumn semester; PHY 301 (Atomic and Molecular Physics); Integrated PhD; 12 students; with 1 (Prof. Anjan Barman) co-teacher
2. Autumn semester; CB 527 (Molecular Physics & Spectroscopy); PhD; 1 student; with 1 (Prof. Anjan Barman) co-teacher
3. Autumn semester; PHY 501 (Research Methodology); PhD; 20 students; with 1 (Prof. Atindra Nath Pal) co-teacher
4. Spring semester; PHY 405 (Biological Physics); Integrated PhD; 5 students

Publications

a) In journals

1. Debasish Das Mahanta and **Rajib Kumar Mitra**, *Connection of large amplitude angular jump motions with temporal heterogeneity in aqueous solutions*, Physical Chemistry Chemical Physics, 22, 9339-9348, 2020
2. S Bayan, D Bhattacharya, **R K Mitra** and **S K Ray**, *Self-powered flexible photodetectors based on Ag nanoparticle-loaded g-C_3N_4 nanosheets and*

PVDF hybrids: role of plasmonic and piezoelectric effects, Nanotechnology, 31(36):365401, 2020

3. Didhiti Bhattacharya, Sayan Bayan, **Rajib K. Mitra**, and **Samit K. Ray**, *Flexible Biomechanical Energy Harvesters with Colossal Piezoelectric Output (2.07 V/kPa) Based on Transition Metal Dichalcogenides-Poly(vinylidene fluoride) Nanocomposites*, ACS Applied Electronic Materials, 2, 3327 – 3335, 2020
4. S. Bayan, D. Bhattacharya, **R. K. Mitra** and **S. K. Ray**, *Two-dimensional graphitic carbon nitride nanosheets: a novel platform for flexible, robust and optically active triboelectric nanogenerators*, Nanoscale, 12, 21334 – 21343, 2020
5. Sk Imadul Islam, Arindam Das and **Rajib Kumar Mitra**, *Excited state proton transfer in reverse micelles: Effect of temperature and a possible interplay with salvation*, Journal of Photochemistry and Photobiology A: Chemistry, 404, 112928, 2021
6. Partha Pyne, Nirnay Samanta, Himanshu Gohil, S. S. Prabhu and **Rajib Kumar Mitra**, *Alteration of water absorption in the THz region traces the onset of fibrillation in proteins*, Chemical Communications, 57, 998 – 1001, 2021

Administrative duties

1. Faculty in-charge, students affairs
2. Member, Admission committee
3. Chairman, Internal Standing Technical Committee; Convener, External Technical Committee
4. Member, Students' Curriculum & Research Evaluation (SCREC) Committee
5. Warden, Students hostel

Extramural Projects (DST, CSIR, DAE, UNDP, etc.)

1. Application of TeraHertz Spectroscopy to Membrane Hydration Dynamics, Complemented by Time Resolved Fluorescence Approaches; CSIR; 2019-2022; PI
2. Investigation on the Changes in Protein Hydration During Aggregation in Crowded Environment by THz Time Domain and Optical Time Resolved Spectroscopy; SERB-DST; 2020-2023; PI

Scientific collaborations with other national / international institutions (based on joint publications)

1. Collaboration with Prof. S S Prabhu at TIFR, Mumbai; Sl. No. 6; National

Areas of Research

Experimental biophysical chemistry, spectroscopy

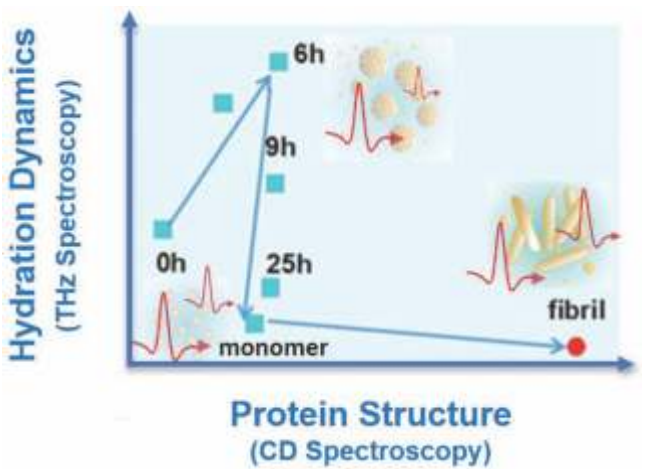
Considering the heterogeneity existing in real biological environments we investigate the excited state proton transfer (ESPT) process in a bio-mimicking reverse micellar (RM) systems. We have made a detailed study on the ESPT process of a photo-acid-luciferin at different temperatures in RMs composed of: anionic AOT, cationic DDAB, and neutral Igepal-520 using steady state and time resolved fluorescence measurements. We found that with increasing temperature both solvation as well as the ESPT rate accelerate, however, the extent of the increase is RM specifc, and they even not complement each other. Our study has established the pivotal role of solvation to be considered to explain ESPT process, specially in constrained environments like in RMs.

We have made a simulation investigation on the large angular jumps that take place when a rotating water molecule exchanges its hydrogen bond (H-bond) identity. This motion differs from the small angular diffusional steps occurring within short time intervals which define the 'Debye diffusion model' of water dynamics. Our investigation was intended to whether these two processes do eventually complement each other. Orientational dynamics of water in its mixture with a small hydrophobic molecule 1,2-dimethoxy ethane (DME) was studied microscopically using the all-atom classical molecular dynamics (MD) simulation technique. We found that the reorientational motions of water molecules are governed by continuous making and breaking of intermolecular H-bonds with their partners. We characterise these H-bond reorientation motions with the description of the ''large amplitude angular jump model'' and explore the coupling between the rotational

and translational motions. By following the trajectories of each molecule in the solutions we describe the orientational dynamics of liquid water with a 'continuous time random walk' (CTRW) approach. Finally, we explored the diffusivity distribution through the jump properties of the water molecules, which successfully leads to the inherent transient heterogeneity of the solutions. We observed that the heterogeneity increases with increasing DME content in the mixtures. Our study correlates the coupling between rotational and translational motions of water molecules in the mixtures.

A scalable, flexible, cost-effective self-poled piezoelectric nanogenerator was fabricated by using chemically exfoliated layered MoS_2 nanosheets embedded in poly (vinylidene fluoride) PVDF polymers. This nanogenerator was able to produce 22V under 10.6kPa mechanical impact leading to an unprecedented piezoelectric output (2.07 V/kPa) using a two-dimensional materials, as well as was able to generate piezoelectric output voltage by mechanical bending via strain, with a piezoelectric energy conversion efficiency of ~ 17.8%, which was capable to drive multiple commercial light emitting devices. It also appeared as an excellent bio-mechanical energy harvesting device which offers an excellent power density of ~88.5 $\mu W/cm^2$ upon finger tapping (~3.1 kPa).

Using terahertz spectroscopy, we established the alteration of the collective hydration of water during the fibrillation process (native - intermediate - fibril) of a model protein bovine serum albumin. This is one of the very first reports on the dynamics of water during fibril formulation. The label-free THz study concludes that water dynamics change systematically with protein conformational changes as it experiences a hydrophobic environment during the initial protein unfolding process, followed by the release of bound water during oligomerization and finally the hydrophobic interior of the fibril. Our study unambiguously concluded a strong correlation between the change in hydration (as obtained from THz spectroscopy) and the structural perturbation (as evidenced from the CD signal) as two clear transitions were observed in the fibrillation pathways. Such in vitro study is a primary step towards experimentally detecting the onset of the fibrillation process via THz spectroscopy of the water network structure.



Plan of Future Work Including Project

1. We plan to underline the inherent role of solvation dynamics on the excited state proton transfer (ESPT) process of some photo-acids. We would use various solvents of different polarities and their mixtures (both in bulk and encapsulated in reverse micelles) and would apply two different time-resolved techniques (fluorescence and transient absorption) to accomplish this.
2. Fabrication of efficient flexible photosensitive piezoelectric nanogenerators (PENG) using composites of polyvinylidene fluoride (PVDF) and chemically exfoliated tungsten disulfide (WS2) nanosheets. Such device is expected to produce an enormously high output voltage compared to the conventional ones. We will also explore photo-response of such materials.
3. We would continue our study to understanding how molecular crowders (salts, amino acids, solvents etc.) interact with biomolecules and affect their biological activity. Such molecular crowders often mimic the real cellular environments. We pay special reference to the effect of various ionic liquids on protein stability. We will make a detailed spectroscopic as well as thermodynamic analysis of the processes involved using differential scanning calorimetry measurements. This study will include both experimental as well as simulation measurements.

4. We plan to combine two experimental approaches namely THz time domain spectroscopy (which probes the low frequency collective vibration models of water, and therefore very sensitive to the global network dynamics of water around hydrophobic surfaces) and optical pump-probe (transient absorption) spectroscopy (which is extremely sensitive to the local environment of a chromophore) to monitor the expected change in overall hydration of a protein during their self-aggregation. The results of this proposed work would render positive impetus for advancement in the research on the protein-aggregation based neurodegenerative diseases. Among the self-aggregated systems we would study protein aggregation (with a special reference to liquid-liquid phase separation in proteins), fibril formation and on amphiphilic self-aggregates like micelles, vesicles, liposomes etc.

5. We plan to explore the effect of cholesterol and its biosynthetic precursors on hydration dynamics in membranes and vesicles of different phases and its implications in the complex, evolutionarily fine-tuned biology of cholesterol in membranes and vesicles using THz spectroscopy complemented by time resolved fluorescence approaches. Insights obtained from the proposed experiments would provide with fundamental knowledge in membrane hydration dynamics that could be relevant in the context of various membrane phenomena such as membrane fusion and regulation of lipid-protein interactions in a membrane milieu. We also plan to carry out atomic force microscopy measurements on vesicles (made by lipids and surfactants) in absence and in presence of cholesterol to underline the elastic properties of the interface.