

Suman Chakrabarty

Associate Professor
CBMS
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Guidance of Students/Post-Docs/Scientists

a) Ph.D. Students

1. Abhinandan Das; Rational design and mechanism of action of potent inhibitors for Acetylcholinesterase enzyme; Under progress
2. Krishnendu Sinha; Phosphorylation code in RhoGDI regulation; Under progress
3. Shounak Mukherjee; Molecular mechanism of ion pumping by KR2 Rhodopsin; Under progress

b) Post-Docs

1. Ipsita Basu; Understanding the role of protein-membrane interactions towards function of GPCR class of proteins

Teaching

1. Autumn semester; Numerical Methods (CB 521); PhD; 20 students

2. Spring semester; Study of BioMacromolecules (CB 540); PhD; 3 students; with 1 (Dr. Tatini Rakshit) co-teacher

Publications

a) In journals

1. Amit Kumawat and **Suman Chakrabarty**, *Protonation-Induced Dynamic Allostery in PDZ Domain: Evidence of Perturbation-Independent Universal Response Network*, *The Journal of Physical Chemistry Letters*, 11, 9026 – 9031, 2020
2. Sinjan Das, Shounak Mukherjee, **Suman Chakrabarty**, and Nitin Chattopadhyay, *Hydroxyl Group-Directed Solvation of Excited-State Intramolecular Proton Transfer Probes in Water: A Demonstration from the Fluorescence Anisotropy of Hydroxyflavones*, *The Journal of Physical Chemistry A*, 125, 57 – 64, 2021
3. Amit Kumawat, Shabnam Raheem, Fasil Ali, Tanveer Ali Dar, **Suman Chakrabarty**, Masood Ahmad Rizvi, *Organoselenium Compounds as Acetylcholinesterase Inhibitors: Evidence and Mechanism of Mixed Inhibition*, *The Journal of Physical Chemistry B*, 125, 1531 – 1541, 2021
4. Prayasee Baruah, Abhinandan Das, Debojit Paul, **Suman Chakrabarty**, Kripamoy Aguan, and Sivaprasad Mitra, *Sulfonylurea Class of Antidiabetic Drugs Inhibit Acetylcholinesterase Activity: Unexplored Auxiliary Pharmacological Benefit toward Alzheimer's Disease*, *ACS Pharmacology & Translational Science*, 4, 193-205, 2021
5. Nilesh Choudhary, Omkar Singh Kushwaha, Gaurav Bhattacharjee, **Suman Chakrabarty**, and Rajnish Kumar, *Macro and Molecular Level Insights on Gas Hydrate Growth in the Presence of Hofmeister Salts*, *Industrial & Engineering Chemistry Research*, 59, 20591 – 20600, 2020
6. Vrushali Hande, Nilesh Choudhary, **Suman Chakrabarty** and Rajnish Kumar, *Morphology and dynamics of self-assembled structures in mixed surfactant systems (SDS + CAPB) in the context of methane hydrate growth*, *Journal of Molecular Liquids*, 319, 114296, 2020

b) Conference proceedings / Reports / Monographs / Books

1. Suman Chakrabarty, "Role of Buried Water in the Mechanism of Photoactivation of KR2 Rhodopsin" *Biophysical Journal* 120, 131a (2021)

Talks / Seminars Delivered in reputed conference/institutions

1. Statistical Mechanics in Chemistry and Biology (SMCB-2021); Jan 23, 2021; Online 4 days
2. Departmental seminar at Chemistry Department, IIT Gandhinagar; Mar 19, 2021; Online; 1 day

Administrative duties

1. Served in several purchase related committees and student evaluation committees

Membership of Learned Societies

1. Biophysical Society, USA
2. American Chemical Society (ACS), USA

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

1. Molecular mechanism of regulation of Rho GTPases through phosphorylation of RhoGDI: Towards unraveling the "phosphorylation code"; SERB, DST, India; 3 years; PI

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

1. Collaboration with Prof. Nitin Chattopadhyay from Jadavpur University on the microscopic origin of high fluorescence anisotropy for Hydroxyflavones; Molecular mechanism of ion pumping by KR2 Rhodopsin; National
2. Collaboration with Prof. M. A. Rizvi from University of Kashmir on the mechanism and role of organoselenium compounds as Acetylcholinesterase inhibitors; Sl. No. 3; National

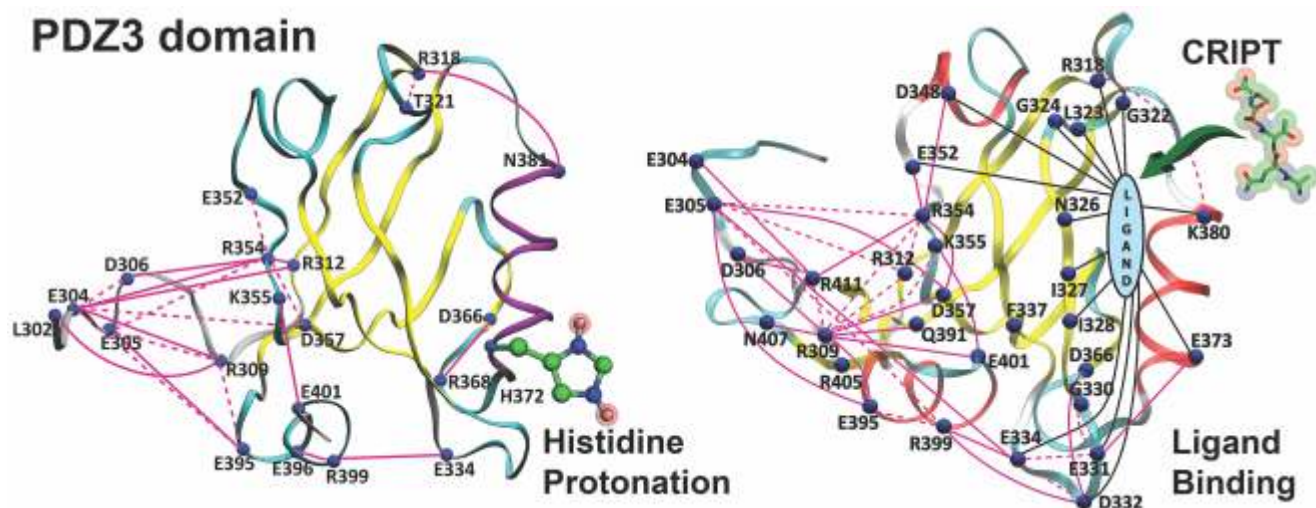
3. Collaboration with Prof. Sivaprasad Mitra from North-Eastern Hill University (NEHU) on the mechanism and role of sulfonylurea class of antidiabetic drugs as Acetylcholinesterase inhibitors; Study of BioMacromolecules (CB 540); National
4. Collaboration with Prof. Rajnish Kumar from IIT Madras on the effect of additives like salts and surfactants on methane hydrate growth kinetics; Sl. No. 5, 6; National

Areas of Research

Theoretical and computational physical chemistry, computational molecular biophysics

We use a combination of large scale atomistic molecular dynamics simulation and enhanced sampling methods to understand the connection between structure, interaction, dynamics and function of complex biomolecular systems. A few representative examples where we have made significant progress recently are:

1. **Universal mechanism of dynamic allostery in PDZ domain:** PDZ domain protein demonstrates a classic example of dynamic allostery, where distal dynamics of side-chains gets modulated on ligand binding without discernible structural changes. Traditionally dynamic allostery has been attributed to purely entropic origin. We have demonstrated earlier (PNAS 2017) that dynamic allostery in PDZ domain can be attributed to long range re-arrangement and re-wiring of hydrogen bonded network and redistribution of electrostatic energies. Recently, we have demonstrated that a different energetic perturbation, namely protonation of a key histidine residue (His372) can also lead to similar dynamic response as ligand binding. Interestingly, the same set of residues seem to be involved. This observation suggests that such proteins may have evolved a unifying universal response system involving hydrogen bonded network that can respond to different types of external perturbations. (Publication: *J. Phys. Chem. Lett.* 11, 9026 (2020)).



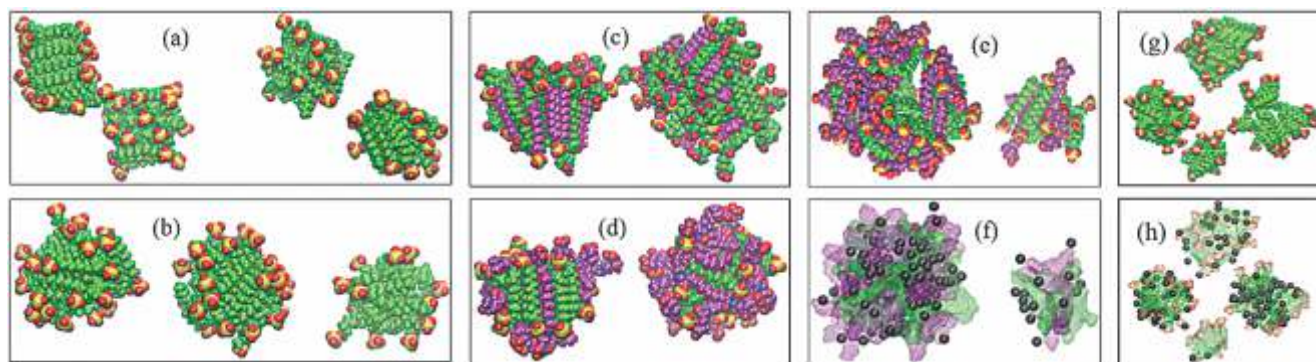
2. **Effect of various additives on the growth kinetics of methane hydrates and the molecular mechanism:**

Marine gas hydrates are promising source of alternative energy. It is crucial to design novel thermodynamic and kinetic promoters of hydrate decomposition for more energy efficient extraction of methane from marine hydrates. Moreover, hydrate formation can have disastrous consequence in fuel pipelines due to blockage. In such scenario, hydrate inhibitors are indispensable. In collaboration with the group of Prof. Rajnish Kumar in IIT Madras, we have investigated the effect of various novel additives on hydrate growth kinetics and developed molecular level understanding of the physico-chemical processes by which such additives function.

(Publications: J. Mol. Liq. 319, 114296 (2020), Ind. Eng. Chem. Res. 59, 20591 (2020))

3. **Inhibition of Acetylcholinesterase (AChE) activity towards therapeutic strategy to control Alzheimer's disease:**

Inhibition of the enzyme Acetylcholinesterase has emerged as a potential strategy to reduce the symptoms of Alzheimer's disease. In collaboration with synthetic chemists we have investigated the molecular mechanism of binding and inhibitory effect of several anti-diabetic drugs and organoselenium compounds on AChE. We have elucidated the origin of experimentally observed mixed inhibition for several of these potential drug molecules. (Publications: ACS Pharmacol. Transl. Sci. 4, 193 (2021), J. Phys. Chem. B 125, 1531 (2021))



Plan of Future Work Including Project

1. Energetics and dynamics of various steps in the photo-activation of Rhodopsin class of proteins. It would involve a combination of QM/MM multi-scale modelling approach as well as enhanced sampling methods like metadynamics and transition path sampling.
2. Development of Markov State Models (MSM) towards elucidating the thermodynamics and kinetics of biomolecular recognition and signalling processes.

Any other Relevant Information including social impact of research

1. The collaborative work with Prof. Rajnish Kumar

on the effect of surfactant mixtures on methane uptake during hydrate formation has been widely discussed and appreciated in the popular media. Some of these are mentioned here:

1. DST media cell: <https://dst.gov.in/newly-designed-additive-molecules-may-obviate-need-long-pipelines-transporting-natural-gas>
2. Tweet by Dr. Harsh Vardhan: <https://twitter.com/drharshvardhan/status/1314792894327267329?lang=en>
3. The Hindu Business Line: <https://www.thehindubusinessline.com/news/science/indian-scientists-discover-chemicals-to-help-make-gas-hydrates-faster/article32918521.ece>