Prof. Rajarshi Chakrabarti (he/his/him)

Contact Information

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Home Page

Web of Science ResearcherID: G-1108-2011
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IRINS Profile
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Current Position

Professor

Personal Information

Date of birth: 17 May 1979
Place of Birth: Kolkata, India
Nationality: Indian
Marital Status: Married with two children
Language: English, Bengali
Fully vaccinated with COVISHIELD on 28 August 2021, Precaution dose on 11 June, 2022

Education

Indian Institute of Science,
Department of Inorganic and Physical Chemistry
Bangalore, India

Ph. D. , Submitted: 2008, Awarded: 2009

- Dissertation Topic: "Statistical Mechanical models of some condensed phase rate processes"
- Advisor: K. L. Sebastian

University of Calcutta, Kolkata, West Bengal, India

- M.Sc., Chemistry, 2003 (Specialization: Physical Chemistry), **First Class**

Scottish Church College, Kolkata, West Bengal, India

- B.Sc., Chemistry (Hons.), Mathematics and Physics (General), 2001, **First Class**

Research Area

Theoretical Physical Chemistry and Chemical Physics, Biophysical Chemistry, Statistical Mechanics, Soft and Living Matter

Teaching

Theory Courses: Physical Chemistry (CH 107), Statistical Mechanics (CH 576), Molecular Energetics and Dynamics (CH 408), Fundamentals of Molecular Energetics and Dynamics (CH 814), Topics in Chemistry (CH 826), Chemical Bond and Molecular Geometry (CH 425), Computational Chemistry (CH 504).

Lab Courses: CH 433, CH 434, CH 117, CH 831 (see IIT Bombay Chemistry website for details).

Taught the students in the National Initiative for Undergraduate Sciences (NIUS) Chemistry camps, organized by the Homi Bhaba Centre for Science Education (HBCSE).

Current Research interests

We cherish in developing statistical mechanical models and applying them to investigate a wide range of interesting problems in physical chemistry, biophysical chemistry, chemical physics, soft and living matter. We are also interested in fundamental topics in statistical mechanics. The main theme of research of our group has been "*Elucidation of structure and dynamics of macromolecules in the condensed phase using computer simulations and statistical mechanical theories*". We work independently as well as in close collaboration with experimentalists. We use analytical techniques and computer simulations as tools. Some of our current research interests are:

Passive and active tracer dynamics in crowded environment and in magnetic fluid:

Using molecular dynamics simulations we have investigated the tracer diffusion in a sea of polymers with specific binding zones for the tracer. These binding zones act as traps. Our simulations show that the tracer can undergo normal yet non-Gaussian diffusion under certain circumstances, e.g., when the polymers with traps are frozen in space and the volume fraction and the binding strength of the traps are moderate. In this case, as the tracer moves, it experiences a heterogeneous environment and exhibits confined continuous time random walk (CTRW) like motion resulting in a non-Gaussian behavior. Also the long time dynamics becomes subdiffusive as the number or the binding strength of the traps increases. However, if the polymers are mobile then the tracer dynamics is Gaussian but could be normal or subdiffusive depending on the number and the binding strength of the traps. In addition, with increasing binding strength and number of polymer traps, the probability of the tracer being trapped increases. On the other hand, removing the binding zones does not result in trapping, even at comparatively high crowding. Our simulations also showed that the trapping probability increases with the increasing size of the tracer and for a bigger tracer with the frozen polymer background the dynamics is only weakly non-Gaussian but highly subdiffusive. Our observations are in the same spirit as found in many recent experiments on tracer diffusion in polymeric materials and question the validity of using Gaussian theory to describe diffusion in a crowded environment in general. More recently, our group has worked on the tracer diffusion in polymer gel and in particular how size, shape of the tracer and the flexibility of the gel affect the dynamics and in particular on the emergence of non-Gaussian heavy tailed dynamics of the probe. In addition, we are currently investigating the dynamics of active Janus probe in crowded environment and the decoupling of its translational-rotational dynamics as observed at moderate crowding. Another related topic of research is controlling the diffusion of nanosized non-magnetic active particle in a magnetic fluid by external magnetic field.

Fluctuation relations and entropy production in active medium:

A colloidal particle immersed in a bath of bacteria is a typical example of a passive particle in an active bath. To model this, we take an overdamped harmonically trapped particle subjected to a thermal and a non-equilibrium noise arising from the active bath. The harmonic well can be attributed to a laser trap or to the small amplitude motion of the sedimented colloid at the bottom of the capillary. In the long time, the system reaches a non-equilibrium steady state that can be described by an effective temperature. Here we

investigate whether fluctuation relations for entropy hold in the presence of Gaussian active noise. In addition, when subjected to a deterministic time dependent drag, we find that transient fluctuation theorem for work cannot be applied in conventional form. However, a steady state fluctuation relation for work emerges out with a renormalized temperature. More recently we have quantified the entropy production in active bath in terms of a time dependent active temperature of the medium.

Theory of active polymers and Structural Organization of Chromatin:

In a typical single molecule experiment, the dynamics of an unfolded protein is studied by determining the reconfiguration time using long-range Förster resonance energy transfer, where the reconfiguration time is the characteristic decay time of the position correlation between two residues of the protein. We have theoretically calculated the reconfiguration time for a single flexible polymer in the presence of active noise. The study suggests that though the mean square displacement grows faster, the chain reconfiguration is always slower in the presence of long-lived active noise with exponential temporal correlation. Similar behavior is observed for a worm-like semiflexible chain and a Zimm chain. However it is primarily the characteristic correlation time of the active noise and not the strength that controls the increase in the reconfiguration time. In brief, such active noise makes the polymer move faster but the correlation loss between the monomers becomes slow. More recently we have analyzed the dynamics of the tagged monomer subjected to a Gaussian as well as a non-Gaussian active noise. An intermediate time superdiffusive motion emerges due to activity.

A living cell is an active environment where the organization and dynamics of chromatin are affected by different forms of activity. Optical experiments report that loci show subdiffusive dynamics and the chromatin fiber is seen to be coherent over micrometer-scale regions. Using a bead-spring polymer chain with dipolar active forces, we study how the subdiffusive motion of the loci generate large-scale coherent motion of the chromatin. We show that in the presence of extensile (contractile) activity, the dynamics of the loci grows faster (slower) and the spatial correlation length increases (decreases) compared to the case with no dipolar forces. Hence, both the dipolar active forces modify the elasticity of the chain. Interestingly in our model, the dynamics and organization of such dipolar active chains largely differ from the passive chain with renormalized elasticity.

Peptide-protein interaction:

Peptide-protein interaction is one of the key regulatory features driving biomolecular processes and hence is targeted for designing therapeutics against diseases. Small peptides are a new and emerging class of therapeutics owing to their high specificity and low toxicity. For achieving efficient targeting of the PPI, amino acid side chains are often stapled together, resulting in the rigidification of these peptides. Exploring the scope of these peptides demands a comprehensive understanding of their working principle. In this work, two stapled p53 peptides have been considered to delineate their binding mechanism with mdm2 using computational approaches. The addition of stapling agent protects the secondary structure of the peptides even in the case of thermal and chemical denaturation. Although the introduction of a stapling agent increases the hydrophobicity of the peptide, the enthalpic stabilization decreases. This is overcome by the lowering of the entropic penalty, and the overall binding affinity improves. The mechanistic insights into the benefit of peptide stapling can be adopted for further improvement of peptide therapeutics.

Counteraction of ammonium-based ionic liquid and Choline Chloride to urea-induced denaturation of proteins:

Recently, room temperature ionic liquids (ILs) have been shown to counteract the deleterious effect of urea on proteins. Using atomistic molecular dynamics we show that a ternary mixture containing a particular 20 ammonium-based IL, triethylammonium acetate (TEAA), and urea, the folding/unfolding equilibrium of proteins in an aqueous medium can be altered by adding small organic molecules generally termed as co-solvents. Denaturants such as urea are instrumental in the unfolding of proteins while protecting osmolytes favor the folded ensemble (1 : 5 molar ratio) helps a small 15- residue S-peptide analog regain most of its native structure, whereas a binary aqueous mixture containing a large amount of urea alone completely distorts it. Our simulations show that the denaturant urea directly interacts with the peptide backbone in the binary mixture while for the ternary mixture both urea as well as the IL are preferentially excluded from the peptide surface. Similar observation for Choline chloride and we have analyzed the phenomenon in detailed, focusing on the hydrogen bond and rotational dynamics of choline chloride.

Internal friction and polymer dynamics:

Loop formation in long chain molecules is a primary step in polypeptide, protein folding as well as in processes like DNA transcription. We have recently looked at the effect of hydrodynamic interaction on end-to-end loop formation in flexible polymer. We have shown how hydrodynamics can actually make loop formation faster. On the other hand, in a separate study, we have shown that the presence of viscoelastic solvent around the chain makes looping dynamics slow. Very recently we have analyzed how internal friction can influence end-to-end looping dynamics. We have also analyzed how fluctuating hydrodynamics in addition to internal viscosity affect the dynamics in a dumbbell model for polymer chain. Our recent work dealt with the use of Jarzynski equality to measure the internal friction of a polymer from optical tweezer experiments. A future problem would be to come up with a multi-chain code to model real dilute polymer solution and investigate the combined effect of hydrodynamics and internal viscosity on dynamics.

Honors, Awards and Additional Responsibilities

Graduate Aptitude Test in Engineering (GATE 2003), conducted by Indian Institute of Technology (IIT), **percentile score: 98.71, all India rank 34**.

Junior Research Fellowship and eligibility for lectureship (2003-2005) awarded by the Council of Scientific and Industrial Research (CSIR) on the basis of an all India Examination.

Senior Research Fellowship (2005-2008), awarded by the Council of Scientific and Industrial Research (CSIR) on the basis of the research done as the Junior Research Fellow.

IIT Bombay Young Faculty Award 2013.

IIT Bombay Early Research Achiever Award 2016.

Departmental Excellence in teaching award 2020.

Microsoft Azure Cloud and High-Performance Computing award from COVID-19 HPC Consortium.

Visiting Scientist: Max Planck Institute for Physics of Complex System, Dresden, 28 February- 30 April 2019.

Visiting Scientist: Max Planck Institute for Physics of Complex System, Dresden, 1 May- 10 June 2022.

Visiting Collaborator: Soft Matter and Computational Physics Group, University of

Vienna, 30 May - 4 June 2022.

IOP Publishing Top Cited Author Award (India) in Mathematical Sciences for the article: Chain reconfiguration in active noise.

Achieved: IOP trusted reviewer status.

Fellow of Indian Chemical Society (FICS), 2019.

Associate Editor: Biophysics - Frontiers, a specialty section within frontiers in Physics, frontiers in Physiology and frontiers in Molecular Biosciences (March 2020 -).

Editorial Board Member: Journal of Physics A: Mathematical and Theoretical (April 2023 -).

Associate Editor: International Journal of Chemical Kinetics, Wiley (June 2020 - December 2023).

Member: International Advisory Board, Journal of the Indian Chemical Society (January 2021 -).

Guest Editor: Frontiers in Physics - Rising Stars Asia (2020).

Member: Chemical Research Society of India (CRSI) (Membership No: LM 2314).

Member: American Physical Society (APS).

Member: American Chemical Society (ACS).

Work Experience

Professor **May 2021 -**

Department of Chemistry
Indian Institute of Technology Bombay

Associate Professor **December 2016 - May 2021**

Department of Chemistry
Indian Institute of Technology Bombay

Assistant Professor **January 2013 - November 2016**

Department of Chemistry
Indian Institute of Technology Bombay

Post Doctoral Research Associate **June 2011 - December 2012**

Institute for Computational Physics
University of Stuttgart, Stuttgart, Germany

Advisor: Christian Holm

Research: Theory and molecular dynamics simulation of diffusion of tracer particles through

crowded cylindrical channel.

Research Associate **January 2011 - May 2011**

Department of Inorganic and Physical Chemistry
Indian Institute of Science, Bangalore, India

Advisor: K. L. Sebastian

Research: Theory of end to end loop formation in flexible polymer in presence of hydrodynamic interaction and in viscoelastic fluid.

Post Doctoral Research Associate **February 2009 - January 2011**

Department of Materials Science and Engineering
University of Illinois at Urbana Champaign, Urbana, USA

Advisor: Kenneth S Schweizer

Research: Theoretical investigation of polymer nanoparticle mixture and fractal like aggregates in equilibrium and dynamics using liquid state and mode coupling theory in close collaboration with **Michelin** (France).

PUBLICATIONS FROM IIT BOMBAY

- **67.** Mechanism of Deamination of Mycobacterial Deaminase Selectively Targeting Mutagenic Bases - Sini Porathoor, Asha Rani Choudhury, **Rajarshi Chakrabarti** and Ruchi Anand (submitted).
- **66.** Osmolyte-induced Conformational Stabilization of a Hydrophobic Polymer - Pooja Nanavare, Soham Sarkar, Abhijit Bijay Jena and **Rajarshi Chakrabarti** (submitted).
- **65.** Exploring the Effect of Hydrocarbon Crosslinkers on the Structure and Binding of Stapled p53 Peptide - Asha Rani Choudhury, Vikram Gaikwad, Atanu Maity and **Rajarshi Chakrabarti** (submitted).
- **64.** A Passive Star Polymer in a Dense Active Bath: Insights from Computer Simulations - Ramanand Singh Yadav, Sanaa Sharma, Ralf Metzler and **Rajarshi Chakrabarti** *Soft Matter* xx, xxxx (2024).
- **63.** Decoding the Dynamics of BCL9 Triazole Stapled Peptide - Vikram Gaikwad, Asha Rani Choudhury and **Rajarshi Chakrabarti** *Biophys. Chem.* 307, 107197 (2024).
- **62.** Dynamic Clustering of Active Rings - Ligesh Theeyancheri, Subhasish Chaki, Tapomoy Bhattacharjee and **Rajarshi Chakrabarti** *Phys. Rev. Res.*, 6, L012038 (2024).
- **61** Escape dynamics of a self-propelled nanorod from circular confinements with narrow openings - Praveen Kumar and **Rajarshi Chakrabarti** *Soft Matter* 19, 6743 (2023).
- **60.** Structure and dynamics of an active polymer chain inside a nanochannel grafted with polymers - Rajiblochan Sahoo and **Rajarshi Chakrabarti** *Soft Matter* 19, 5978 (2023).
- **59.** Active Dynamics of Linear Chains and Rings in Porous Media - Ligesh Theeyancheri, Subhasish Chaki, Tapomoy Bhattacharjee and **Rajarshi Chakrabarti** *J. Chem. Phys.* 159, 014902 (2023).

- **58.** Dynamics of a Methane Hydrophobe in Aqueous Choline Chloride Solution: Insights from Molecular Dynamics Simulations - Pooja Nanavare, Ligesh Theeyancheri, Soham Sarkar and **Rajarshi Chakrabarti** *Chem. Phys. Impact.* 6, 100223 (2023).

- **57.** A Polymer Chain with Dipolar Active Forces in Connection to Spatial Organization of Chromatin - Subhasish Chaki, Ligesh Theeyancheri, and **Rajarshi Chakrabarti** *Soft Matter* 19, 1348 (2023).

- **56.** Dynamics of a spherical self-propelled tracer in a polymeric medium: interplay of self-propulsion, stickiness, and crowding - Ramanand Singh Yadav, Chintu Das and **Rajarshi Chakrabarti** *Soft Matter* 19, 689 (2023).

- **55.** Dynamics of self-propelled tracer particles inside a polymer network - Praveen Kumar and **Rajarshi Chakrabarti** *Phys. Chem. Chem. Phys.* 25, 1937 (2023).

- **54.** Shear viscosity for finitely extensible chains with fluctuating internal friction and hydrodynamic interactions - R. Kailasham, **Rajarshi Chakrabarti** and J. Ravi Prakash *J. Rheology*, 67, 105 (2023).

- **53.** Reconfiguration, swelling and tagged monomer dynamics of a single polymer chain in Gaussian and non-Gaussian active baths - Koushik Goswami, Subhasish Chaki and **Rajarshi Chakrabarti** *J. Phys. A: Math and Theo.*, 55, 423002 (2022). **Invited Topical Review**.

- **52.** In Silico Studies of Active Probe Dynamics in Crowded Media - Ligesh Theeyancheri, Rajiblochan Sahoo, Praveen Kumar and **Rajarshi Chakrabarti** *ACS Omega*, 7, 33637 (2022). **Invited Mini-Review**.

- **51.** Distinct mode of membrane interaction and disintegration by diverse class of Antimicrobial peptides - Nutan Agadi, Atanu Maity, Akash Kumar Jha, **Rajarshi Chakrabarti** and Ashutosh Kumar *BBA-Biomembranes*, 1864, 184047 (2022).

- **50.** Structure and Orientation of Water and Choline Chloride Molecules Around a Methane Hydrophobe: A Computer Simulation Study - Pooja Nanavare, Asha Rani Choudhury, Soham Sarkar, Atanu Maity and **Rajarshi Chakrabarti** *ChemPhysChem* **23**, e202200446 (2022) (Special Collection Issue: Theoretical Chemistry Symposium 2021). **This article has appeared as a Cover Feature of the Journal.**

- **49.** Migration of active rings in porous media - Ligesh Theeyancheri, Subhasish Chaki, Tapomoy Bhattacharjee and **Rajarshi Chakrabarti** *Phys. Rev. E.* **106**, 014504 (2022).

- **48.** Computational design of stapled peptide inhibitor against SARS CoV-2 receptor binding domain - Asha Rani Choudhury, Atanu Maity, Sayantani Chakraborty and **Rajarshi Chakrabarti** *Peptide Science* **e24267** (2022).

- **47.** Chemically symmetric and asymmetric self-driven dumbbells in 2D polymer gel - Praveen Kumar, Ligesh Theeyancheri, and **Rajarshi Chakrabarti** *Soft Matter* **18**, 2663 (2022).

- **46.** Motion of an active particle with dynamical disorder - Koushik Goswami, and **Rajarshi Chakrabarti** *Soft Matter* **18**, 2332 (2022).

- **45.** Transport of a self-propelled tracer through a hairy cylindrical channel: interplay of stickiness and activity - Rajiblochan Sahoo, Ligesh Theeyancheri and **Rajarshi**

Chakrabarti *Soft Matter* **18**, 1310 (2022).

- **44.** In silico Elucidation of Molecular Picture of Water-Choline Chloride Mixture - Soham Sarkar, Atanu Maity and **Rajarshi Chakrabarti** *J. Phys. Chem. B* **125**, 13212 (2021).

- **43.** Stochastic resetting and first arrival subjected to Gaussian noise and Poisson white noise - Koushik Goswami and **Rajarshi Chakrabarti** *Phys. Rev. E* **104**, 034113 (2021).

- **42.** How important are fluctuations in the treatment of internal friction in polymers? - R. Kailasham, **Rajarshi Chakrabarti** and J. Ravi Prakash *Soft Matter* **17**, 7133 (2021).

- **41.** Rouse model with fluctuating internal friction - R. Kailasham, **Rajarshi Chakrabarti** and J. Ravi Prakash *J. Rheol.* **65**, 903 (2021).

- **40.** Effect of Stapling Agent on the Thermodynamics of mdm2-p53 Binding - Atanu Maity, Asha Rani Choudhury and **Rajarshi Chakrabarti** *J. Chem. Inf. Model.* **61**, 1989 (2021).

- **39.** Microscopic Structural Features of Water in Aqueous-Reline Mixture of Varying Compositions - Soham Sarkar, Atanu Maity and **Rajarshi Chakrabarti** *Phys. Chem. Chem. Phys.* **23**, 3779 (2021).

- **38.** Directing the diffusion of a non-magnetic nanosized active particle with external magnetic fields - Martin Kaiser, Pedro A. Sanchez, Nairhita Samanta, **Rajarshi Chakrabarti** and Sofia S. Kantorovich *J. Phys. Chem. B* **124**, 8188 (2020).

- **37.** Translational and rotational dynamics of a self-propelled janus probe in crowded environments - Ligesh Theeyancheri, Subhasish Chaki, Nairhita Samanta, Rohit Goswami, Raghunath Chelakkot and **Rajarshi Chakrabarti** *Soft Matter* **16**, 8482 (2020).

- **36.** Escape of a passive particle from activity-induced energy landscape: Emergence of slow and fast effective diffusion - Subhasish Chaki and **Rajarshi Chakrabarti** *Soft Matter* **16**, 7103 (2020). **This article has been featured in an online themed collection: Soft Matter Most Popular 2020.**

- **35.** Wet and dry Internal friction can be measured with the Jarzynski equality - R. Kailasham, **Rajarshi Chakrabarti** and J. Ravi Prakash, *Phys. Rev. Res.* **2**, 013331 (2020).

- **34.** Choline chloride as a nano-crowder protects HP-36 from urea-induced denaturation by preserving the hydration layer: Insights from Solvent Dynamics and Protein-Solvent interaction - Atanu Maity, Soham Sarkar, Ligesh Theeyancheri and **Rajarshi Chakrabarti**, *ChemPhysChem* **21**, 552-567 (2020).

- **33.** Transport of probe particles in polymer network: effects of probe size, network rigidity and probe-polymer interaction - Praveen Kumar, Ligesh Theeyancheri, Subhasish Chaki and **Rajarshi Chakrabarti**, *Soft Matter* **15**, 8992 (2019). **This article has appeared as a back cover page of the Journal.**

- **32.** Effects of active fluctuations on energetics of a colloidal particle: superdiffusion, dissipation and entropy production - Subhasish Chaki and **Rajarshi Chakrabarti**, *Physica A* **530**, 121574 (2019).

- **31.** Azadirachtin inhibits amyloid formation, disaggregates pre-formed fibrils, and protects pancreatic β-cells from human islet amyloid polypeptide (hIAPP) induced cytotoxicity - Richa Dubey, Ketaki Patil, Sarath Chandra Dantu, Parnika Bhatia, Nikita Malik, Jhankar D. Acharya, Soham Sarkar, Soumadwip Ghosh, **Rajarshi Chakrabarti**, Shilpy Sharma, Ashutosh Kumar, *Biochemical Journal* **476**, 889 (2019).

- **30.** Enhanced diffusion, swelling and slow reconfiguration of a single chain in non-Gaussian active bath- Subhasish Chaki and **Rajarshi Chakrabarti**, *J. Chem. Phys.* **150**, 094902 (2019).

- **29.** Salt Induced Structural Collapse, Swelling and Signature of Aggregation of Two ssDNA Strands: Insights from Molecular Dynamics Simulation - Soham Sarkar, Atanu Maity, Aditya Sarma Phukon, Soumadwip Ghosh and **Rajarshi Chakrabarti** *J. Phys. Chem. B.* **123**, 47 (2019).

- **28.** Rheological consequences of wet and dry friction in a dumbbell model with hydrodynamic interactions and internal viscosity - R. Kailasham, **Rajarshi Chakrabarti** and J. Ravi Prakash, *J. Chem. Phys.* **149**, 094903 (2018). **This article has been selected as a 2018 Editors' Choice article.**

- **27.** Entropy production and work fluctuation relations for a single particle in active bath - Subhasish Chaki and **Rajarshi Chakrabarti**, *Physica A* **511**, 302 (2018).

- **26.** Ammonium-based stabilizers effectively counteract the Urea-conferred denaturation in a small protein: Insights from molecular dynamics simulations - Soham Sarkar, Soumadwip Ghosh and **Rajarshi Chakrabarti**, *RSC Adv.* **7**, 52888 (2017).

- **25.** Can ammonium based room temperature ionic liquid counteract the urea induced denaturation of a small peptide? - Soumadwip Ghosh, Souvik Dey, Mahendra Patel and **Rajarshi Chakrabarti**, *Phys. Chem. Chem. Phys.* **19**, 7772 (2017). **This article has been featured in an online themed collection: New Frontiers in Indian Research.**

- **24.** Molecular Dynamics Simulation Elucidates the Preferential Binding Affinity of Sodium and Tetramethylammonium Ions for Tetrameric Nafion Unit under Aqueous Conditions - Soumadwip Ghosh and **Rajarshi Chakrabarti**, *RSC Adv.* **6**, 97961 (2016).

- **23.** Tracer Diffusion in a sea of polymers with binding zones: Mobile vs frozen traps - Nairhita Samanta and **Rajarshi Chakrabarti**, *Soft Matter* **12**, 8554 (2016). **This article has been featured in an online themed collection: New Frontiers in Indian Research.**

- **22.** Unzipping of Double Stranded Ribonucleic Acids by Graphene and Single-Walled Carbon Nanotube: Helix Geometry versus Surface Curvature - Soumadwip Ghosh and **Rajarshi Chakrabarti**, *J. Phys. Chem. C* **120**, 22681 (2016).

- **21.** Spontaneous unzipping of Xylonucleic acid on Single-walled carbon nanotube: A computational study - Soumadwip Ghosh and **Rajarshi Chakrabarti**, *J. Phys. Chem. B* **120**, 3642 (2016).

- **20.** Chain reconfiguration in active noise - Nairhita Samanta and **Rajarshi Chakrabarti**, *J. Phys. A: Math and Theo.* **49**, 195601(2016). **This article has been conferred the**

best citation award from India in the field of mathematics published across the whole IOP Publishing portfolio in the past three years (2016 to 2018).

- **19.** Probing the salt concentration dependent nucleobase distributions in a single stranded DNA-single walled nanotube hybrid with molecular dynamics - Soumadwip Ghosh, Nisheet Patel and **Rajarshi Chakrabarti**, *J. Phys. Chem. B*, **120**, 455 (2016). (Correction: *J. Phys. Chem. B* **120**, 2868 (2016)).

- **18.** Reconfiguration Dynamics in folded and intrinsically disordered protein with internal friction: Effect of solvent quality and denaturant - Nairhita Samanta and **Rajarshi Chakrabarti**, *Physica A* **450**, 165 (2016).

- **17.** Thermodynamics of site specific small molecular ion interaction with DNA duplex : a molecular dynamics study - Soumadwip Ghosh, Mayank K Dixit and **Rajarshi Chakrabarti**, *Mole. Simul.* **42**, 715 (2016).

- **16.** Ion assisted structural collapse of a single stranded DNA: a molecular dynamics approach - Soumadwip Ghosh, Himanshu Dixit and **Rajarshi Chakrabarti**, *Chem. Phys.* **459**, 137 (2015).

- **15.** Looping dynamics of a flexible chain with internal friction at different degrees of compactness - Nairhita Samanta and **Rajarshi Chakrabarti**, *Physica A* **436**, 377 (2015).

- **14.** Looping and reconfiguration dynamics of a flexible chain with internal friction - Nairhita Samanta, Jayanta Ghosh and **Rajarshi Chakrabarti**, *AIP Adv.* **4**, 067102 (2014).

- **13.** Diffusion in an elastic medium: A model for macromolecule transport across the nuclear pore complex - **Rajarshi Chakrabarti**, Ananya Debnath and K. L. Sebastian, *Physica A* **404**, 65 (2014).

- **12.** End to end loop formation in a single polymer chain with internal friction - Nairhita Samanta and **Rajarshi Chakrabarti**, *Chem. Phys. Letts.* **582**, 71 (2013).

- **11.** Tracer diffusion inside a crowded cylindrical channel - **Rajarshi Chakrabarti**, Stefan Kesselheim, Peter Košovan and Christian Holm, *Phys. Rev. E* **87**, 062709 (2013).

Publications Before joining IIT Bombay

- **10.** Dynamics of end-to-end loop formation for an isolated chain in viscoelastic solvent - **Rajarshi Chakrabarti**, *Physica A* **391**, 5326 (2012).

- **9.** Dynamics of end-to-end loop formation: A flexible chain in the presence of hydrodynamic interaction - **Rajarshi Chakrabarti**, *Physica A* **391**, 4081 (2012).

- **8.** Packing Correlations, Collective Scattering and Compressibility of Fractal-like Aggregates in Polymer Nanocomposites and Suspensions - **Rajarshi Chakrabarti**, Jean-Yves Delannoy, Marc Couty and Kenneth S. Schweizer, *Soft Matter* **7**, 5397 (2011).

- **7.** Bubble dynamics in double stranded DNA: A Rouse chain based approach - **Rajarshi Chakrabarti**, *Chem. Phys. Letts.* **502**, 107 (2011).

- **6.** Polymer mediated structure of nanoparticles in dense melts: transferability and effective one component approach - **Rajarshi Chakrabarti** and Kenneth S. Schweizer, *J. Chem. Phys.* **133**, 144905 (2010).

- **5.** Dynamic disorder with exponential sink - **Rajarshi Chakrabarti**, *Chem. Phys. Letts.* **495**, 60 (2010).

- **4.** A lower bound to the survival probability and an approximate first passage time distribution for Markovian and non-Markovian dynamics in phase space - **Rajarshi Chakrabarti** and K. L. Sebastian, *J. Chem. Phys.* **131**, 224504 (2009).

- **3.** Transient state work fluctuation theorem for a classical harmonic oscillator linearly coupled to a harmonic bath - **Rajarshi Chakrabarti**, *Pramana J. Phys.* **72**, 665, (2009).

- **2.** Exact Analytical Evaluation of Time Dependent Transmission Coefficient from the method of reactive flux for an inverted parabolic barrier - **Rajarshi Chakrabarti**, *J. Chem. Phys.* **126**, 134106 (2007).

- **1.** Rate Processes with Dynamical Disorder: A Direct Variational Approach - Ananya Debnath, **Rajarshi Chakrabarti** and K. L. Sebastian, *J. Chem. Phys.* **124**, 204111 (2006).

Conference Proceedings

- **1.** How does the tail length and separation between the tagged monomers influence the reconfiguration of a chain with internal friction for different solvent-quality? - Nairhita Samanta and **Rajarshi Chakrabarti**, *J. Phys: Conf. Ser.* **759**, 012014 (2016).

Conference and Workshops

- Poster presentation in SERC School on Statistical Physics, 2004, TIFR, Mumbai, India.
- STATPHYS 22, 2004, IISc, Bangalore, India.
- DAE-BRNS Symposium on Theoretical Chemistry, BARC, Mumbai, India, 2004.
- ACS-PRF Summer School on Theoretical Chemistry, Utah, USA, 2005.
- Poster presentation in Theoretical Chemistry Symposium 2006, Tiruchirapalli, India.
- Poster presentation in the Conference on Nucleation, Aggregation and Growth, 2007, JNCASR, Bangalore, India.
- Workshop on Jarzynski equality and non-equilibrium fluctuation theorems, 9-12 Feb, 2007, Bangalore, India.
- Poster presentation in Gordon Conference: Liquids, Chemistry and Physics of, 29 July-3 August, 2007, New Hampshire, USA.
- Speaker: Statistical Mechanics Meeting, Bangalore, 2008.
- Speaker: APS March Meeting: Portland, Oregon, USA, March 2010.
- Participation and Poster Presentation in the workshop Coarse-Grained Simulation of Biological Soft Matter Systems using ESPResSo, October 10-14, 2011, Stuttgart, Germany.
- Participation in the Hands-On Workshop on Computational Biophysics in Bremen, October 17-21, 2011, Bremen, Germany.
- Participation in the Hydrogel modeling workshop, November 24-25, 2011, Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany.
- Participation and poster presentation in the tutorial Understanding Molecular Simulation 2012, January 9-20, 2012, University of Amsterdam.
- Speaker: Spring Meeting of the Section Condensed Matter (SKM), 25-30 March 2012, Berlin, Germany.
- Poster presentation in Gordon Conference: Single Molecule Approaches to Biology, 15-20 July, 2012, Vermont, USA.
- Participation in the Workshop Polymer Translocation through Nanopores, Mainz, Germany, September 16-18, 2012.

- Participation in the workshop: Simulating Soft Matter with ESPResSo, ESPResSo++ and VOTCA, 8-12 Oct 2012, Stuttgart, Germany.
- Session Chair: Discussion meeting on Spectroscopy and Dynamics of Molecules and Clusters 2013 (SDMC), 21-24 February 2013, Udaipur, India.
- Session Chair: Symposium on Theoretical and Computational Chemistry: Frontiers and Challenges 2013 (STCC-FC), 14-15 June 2013, Tiruchirapalli, India.
- Session Chair: DAE BRNS Symposium on Current Trends in Theoretical Chemistry (CTTC-2013), 26-28 September 2013, BARC, Mumbai, India.
- Participation: 5 -7 January, 2014, Soft Matter Young Investigators Meet 2014, Puducherry, India.
- Invited Speaker: Discussion meeting on Spectroscopy and Dynamics of Molecules and Clusters 2014 (SDMC), 20-23 February 2014, Puri, India.
- Invited Speaker: 14th Theoretical Chemistry Symposium, 18-21 December 2014, Pune, India.
- Session Chair: Discussion meeting on Spectroscopy and Dynamics of Molecules and Clusters 2015 (SDMC), 19-22 February 2015, Nainital, India.
- Speaker: CompFlu, 1 August 2015, IISER Pune, India.
- Invited Speaker: Anomalous Diffusion: Wild and Bad?, Bad Wildbad, Germany, 4-7 October 2015.
- Invited Speaker: XXVII IUPAP Conference on Computational Physics, CCP2015, IIT Guwahati 2-5 December 2015.
- Invited Speaker: Discussion meeting on Spectroscopy and Dynamics of Molecules and Clusters 2016 (SDMC), 18-21 February 2016, Mahabaleshwar, India.
- Invited Speaker: Recent Advances in Theoretical Chemistry 2016 (RATC 2016), 8-9 July 2016, IISc, Bangalore, India.
- Invited Speaker and Session Chair: Kaleidoscope, a discussion meeting in Chemistry, 13-17 July, 2016, Goa.
- Invited Speaker: Colloquium on Complex and Biological Systems, 18 November 2016, University of Potsdam, Germany.
- Invited Speaker: Computational Physics, 22 November 2016, University of Vienna, Austria.
- Speaker: Department of Physical Chemistry, Indian Association for the Cultivation of Science, Kolkata, 7 December 2016.
- Speaker: CompFlu Hyderabad, 12-14 December, 2016.
- Participation: Theoretical Chemistry Symposium, 14-17 December 2016, Hyderabad, India.
- Speaker: Indian Statistical Physics Community Meeting 2017, International Centre for Theoretical Sciences, Bangalore, 17-19 February, 2017.
- Invited Speaker: DNA Physics, BITS Pilani, 9-11 March, 2017.
- Poster presentation in Gordon Conference: Liquids, Chemistry and Physics of, 6-11 August, 2017, New Hampshire, USA.
- Invited Speaker: Statistical Mechanics of Soft Matter 2017, 27-28 November, 2017, University of Sydney, Australia.
- Speaker: CompFlu Chennai, 18-20 December, 2017.
- Session Chair: Discussion meeting on Spectroscopy and Dynamics of Molecules and Clusters 2018 (SDMC), 15-18 February 2018, Dooars, India.
- Invited Speaker: IACS Conference on Electronic Structure, Spectroscopy and Dynamics (IACS-CESSD 2018), 22-25 February 2018, Kolkata, India.
- Invited Speaker: Emerging trends in Chemical Science, Department of Chemistry, University of Calcutta, 28 March 2018, Kolkata, India.
- Participation and poster presentation in Venice meeting on Fluctuations in small complex systems IV, October 14-18, 2018, Venice, Italy.
- Invited Speaker: 16th Theoretical Chemistry Symposium, 13-16 February 2019, BITS Pilani, India.

- Invited Speaker: Recent Advances in Dynamics at the Interface of Chemistry and Biology (DICB), 18-20 February 2019, Indian Institute of Science, Bangalore, India.
- Speaker: 26 March 2019, Theoretical Physics, University of Potsdam, Germany.
- Speaker: 3 April 2019, MPI PKS Dresden, Germany.
- Speaker: 15 April 2019, Leibniz Institute for Polymer Research Dresden, Germany.
- Session Chair: 12-14 May 2019, Soft Matter Young Investigators Meet 2019, Shillong, India.
- Poster presentation in Gordon Conference: Liquids, Chemistry and Physics of, 4-9 August, 2019, New Hampshire, USA.
- Invited Speaker: 14-15 October 2019, Recent Advances in Chemistry (RAC) 2019, NIT Meghalaya, Shillong, India.
- Invited Speaker: 17 October 2019, S. N. Bose National Centre for Basic Sciences, Department of Chemical, Biological and Macromolecular Sciences, Kolkata, India.
- Invited Visitor and Speaker: 14-15 November 2019, Department of Chemistry, Indian Institute of Technology Kanpur, India.
- Session chair and poster presenter: Modern Approaches in Chemistry and Biology (MACB-2020), 18-20 February, 2020, JNCASR, Bengaluru, India.
- Poster presenter: 20-23 February 2020, Discussion meeting on Spectroscopy and Dynamics of Molecules and Clusters 2020 (SDMC), Kumbhalgarh, India.
- Invited participant: 1-3 March 2020, International Conference on Structure and Dynamics of Molecular and Condensed Matter Systems (ICSD-2020), Puri, India.
- Invited Webinar: 16 July 2020, Faculty Development Program on Recent Advances in Chemical Sciences, SRM Institute of Science and Technology, India.
- Invited Webinar: 28 September 2020, Half Day Virtual Meeting on Theoretical Chemistry at Condensed Phases, Bhabha Atomic Research Centre, India.
- Invited Webinar: 16 November 2020, Department of Chemical Sciences, Tata Institute of Fundamental Research, Mumbai, India.
- Invited Webinar: 30 November 2020, Department of Chemistry, National Institute of Technology Manipur, India.
- Session Chair: 27 December, 2020, 57th Annual Convention of Chemists 2020 and International Conference on Recent Trends in Chemical Sciences (RTCS), Physical Chemistry Section.
- Invited Webinar: 9 January 2021, Discussion meeting on Spectroscopy and Dynamics of Molecules and Clusters (SDMC).
- Invited Webinar: 24 January 2021, Statistical Mechanics in Chemistry and Biology (SMCB), IIT Tirupati-IISER Tirupati (23-26 January 2021).
- Chair: 2 March, 2021, International Webinar Multiscale Simulation and Mathematical Modelling of Complex Biological Systems, Jawaharlal Nehru University.
- Invited Webinar: 13 March 2021, TEQIP-II Sponsored One-Day Seminar on Theoretical and Computational Chemistry, NIT Meghalaya.
- Speaker (virtual mode): APS March Meeting, 15-19 March 2021.
- Speaker (virtual mode): DAE Symposium on Current Trends in Theoretical Chemistry (CTTC-2020), 23-25 September 2021.
- Speaker (virtual mode): Physical Chemistry Physical Biology 2021, 24-28 September 2021.
- Session Chair (virtual mode): Theoretical Chemistry Symposium, 11-14 December 2021, IISER Kolkata.
- Invited Speaker (virtual mode): 22 December 2021, 58th Annual Convention of Chemists and International Conference on Recent Trends in Chemical Sciences, Indian Chemical Society (ICS).
- Invited Speaker (virtual mode): 26 February 2022, IITB-SNBNCBS Interaction Session.
- Speaker (virtual mode): APS March Meeting, 14-18 March 2022.
- Invited Speaker: 7 March 2022, IPC Day, Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bengaluru.

- Invited Speaker (virtual mode): 6 May 2022, Chemical Dynamics in Complex Systems (2022).
- Invited Speaker: 17- 20 May, 2022, Group Retreat Biological Physics, Templin, Germany.
- Invited Speaker (virtual mode): 26 May, 2022, Theoretical Chemistry Meeting: Structure and Dynamics (TCMSD-2022), IACS, Kolkata.
- Speaker: 30 May, 2022, Seminar: Sofia Kantorovich's group, University of Vienna, Austria.
- Invited Speaker: 13 July, 2022, Department of Physics, Indian Institute of Science Education and Research Pune.
- Invited Speaker: Kaleidoscope, a discussion meeting in Chemistry, 28-31 July, 2022, Udaipur.
- Invited Speaker: 17-19 August, 2022, Molecular Biophysics Unit, Indian Institute of Science, Bengaluru.
- Invited Lecturer: 19 August 2022, Molecular Biophysics Unit, Indian Institute of Science, Bengaluru, Lectures of Brownian Motion.
- Invited Speaker: Venice meeting on Fluctuations in small complex systems VI, September 4-9, 2022, Venice, Italy.
- Invited Speaker: 26 October, 2002, Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata.
- Invited Lecturer: 25-28 October, 2022, Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata.
- Poster presenter: 10-13 November 2022, Discussion meeting on Spectroscopy and Dynamics of Molecules and Clusters 20202 (SDMC), Malpe, Karnataka,
- Invited Speaker and Session Chair: 18-20 November 2022. A National Conference on Recent Advances in Chemistry: Theoretical and Computational Aspects, NEHU, Shillong, Meghalaya.
- Invited Speaker: 21 November, 2022, Department of Chemistry, Indian Institute of Technology Guwahati.
- Invited Speaker: 13-14 December, 2022, Molecular Simulation: Focus on Method, TIFR Hyderabad, India.
- Invited Speaker: 5-7 January, 2023, Chennai Soft Matter Days 2023, Indian Institute of Technology Madras.
- Invited Speaker: 5-7 January, 2023, SCS Annual Conference, Indian Association for the Cultivation of Science (IACS), Kolkata.
- Invited Speaker: 9 January, 2023, Department of Physics, IIT Bombay, Interaction Session between IIT Bombay and SNBNCBS, Kolkata.
- Session Chair: 9 February, 2023, One day symposium: Polymers from Physics to Biology organized by Department of Physics, IIT Bombay.
- Invited Speaker: 16-18 March, 2023, Steady State Phenomena in Soft Matter, Active and Biological Systems, S.N. Bose National Center For Basic Sciences, Kolkata.
- Session Chair: 14-17 June, 2023, Soft Matter Young Investigators meet 2023, P.O. Dhela, Jim Corbett National Park, Ramnagar, Uttarakhand, India.
- Invited Speaker: 8-12 August, 2023, International Conference on Soft Matter, Seoul, Korea.
- Invited Speaker: 14-18 August, 2023, International Conference on Biological Physics (ICBP), Seoul, Korea.
- Invited Speaker: 28 August, 2023, Department of Chemistry, Central University of Jammu, India.
- Invited Speaker: 14 September, 2023, "Random Interactions" seminar series in the Department of Theoretical Physics, Tata Institute of Fundamental Research, Mumbai, India.
- Invited Speaker: 5-8 October, 2023, Structure and Dynamics: Spectroscopy and Scattering (SDSS-2023), Indian Association for the Cultivation of Science (IACS), Kolkata.
- Invited Speaker: 29-31 October, 2023: Society of Physical Chemistry Conference, Indian

Institute of Technology Kanpur.

- Invited Speaker; 31 October, 2023: Department of Physics, Indian Institute of Technology Kanpur.
- Invited Speaker: 29 November, 2023: Raman Research Institute, Bengaluru, India.
- Invited Speaker: 7-10 December, 2023: Theoretical Chemistry Symposium (TCS) 2023, Indian Institute of Technology Madras.
- Invited Speaker: 11-14 December, 2023: National Workshop on Atomistic Modeling of Molecules and Materials (AMMM-2023), Chemical Engineering Group, Bhabha Atomic Research Centre (BARC), India.
- Invited Speaker: 14 December, 2023: Symposium on Soft and Biological Materials: Experiments and Theory, Indian Institute of Technology Bombay.
- Invited Speaker: 4-5 January, 2024: Stochastic and Nonlinear dynamics in Chemistry and Biology (SNDCB-2024), S. N. Bose National Centre for Basic Sciences, Kolkata.
- Invited Speaker: 18-20 January, 2024, IGSTC workshop on Engineering for Sustainable and Resilient Development, Indian Institute of Technology Mandi, India.
- Invited Speaker: 19 January, 2024: Department of Chemical Sciences, Indian Institute of Technology Mandi, India.
- Invited Speaker: 1-2 February, 2024, Systems Biology Approaches to Understand Complex Cellular Dynamics (SBAUCCD-2024), Indian Institute of Technology Bombay.
- Invited Contributory Speaker: 5-9 February, 2024, Lorentz workshop - Organization and Dynamics of Active Filaments: From Single Chain to Collectives, Leiden, Netherlands.
- Invited Speaker: 22-25 February, 2024: Spectroscopy and Dynamics of Molecules and Clusters 2024 (SDMC), Kaziranga, Assam, India.
- Invited Speaker: 1 March 2024: One day symposium on Simulation of Physical and Biological Systems at SCIS, JNU, New Delhi, India.
- Speaker: 4-8 March, 2024: APS March Meeting, Minneapolis, USA.
- Speaker: 11 March, 2024: Department of Chemistry, University of Minnesota, USA.

Group Members

Post Docs

Dr. Piyali Mukherjee (Institute postdoctoral fellow, October 2023 -)

Ph. D students

Asha Rani Choudhury (DST-Inspire Fellow, 2018 -) (thesis submitted), **Rajiblochan Sahu** (CSIR Fellow, 2018 -) (thesis submitted), **Ramanand Singh Yadav** (Institute Fellow, 2020 -), **Pooja Nanavare** (UGC Fellow, 2021-), **Rupesh Kumar** (jointly with Rochish Thaokar, Chemical Engineering, IIT Bombay) (PMRF, 2021-), **Arvind** (Institute Fellow, 2022-), **Vikram Gaikwad** (PMRF, 2022-).

M. Sc/B. S students

Abhijit Bijay Jena (2022 -)

Yashit Verma (2023-)

Project students

None

Alumni

Post Docs

Dr. Koushik Goswami (December 2020 - February 2022, Current position: Post Doctoral Researcher, University of Potsdam, Germany)

Dr. Atanu Maity (July 2018 - July 2021, Current position: Project Scientist, Indian Institute of Technology Kharagpur)

PhD students

Dr. Ligesh Theeyancheri (Ph. D., 2018 - 2023) (Current position: Postdoctoral fellow at the Department of Physics, Syracuse University, USA).

Thesis title: **Dynamics and Conformations of Active Agents in Complex Media: From Janus Particles to Linear Chains and Rings**

Dr. Praveen Kumar (Ph. D., 2017 - 2023) (Current position: Postdoctoral fellow at the Department of Physics, Northeastern University, USA).

Thesis title: **Understanding the Dynamics of Active and Passive Probe Particles in Complex Environments using Computer Simulations**

Dr. Subhasish Chaki (Ph. D., 2016 - 2021) (Current position: Humboldt Fellow, Heinrich Heine University, Dusseldorf, Germany).

Thesis title: **Understanding the Activity-Driven Dynamics of Single Colloid and Single Polymer Chain**

Dr. Soham Sarkar (Ph. D., 2016 - 2021) (Current position: Post Doctoral Research Associate, Technical University Darmstadt, Germany).

Thesis title: **Computational Investigations of the Effect of Co-solvents and Ions on the Structure and Dynamics of Water and Biomolecules**

Dr. Kailasham Ramalingam (Ph. D., 2016 - 2021) (Current position: Post Doctoral Research Associate, Carnegie Mellon University, USA, incoming faculty at Indian Institute of Technology Indore).

Thesis title: **The Influence of Internal Friction on Dilute Polymer Solution Dynamics**

Dr. Nairhita Samanta (Ph. D., 2013 - 2018) (Current position: Associate Manager - Data Science, San Francisco, USA), recipient of excellence in Ph. D. thesis award (2018-2020).

Thesis title: **Insights on passive and active dynamics of polymer and colloidal suspensions**

Dr. Soumadwip Ghosh (Ph. D., 2011 - 2017) (Current position: Senior Scientist, Enlaza Therapeutics, San Diego, USA), recipient of excellence in Ph. D. thesis award (2016-2018).

Thesis title: **Investigating the Dynamics of Biomacromolecules in Presence of Excess Salt, Ionic Liquids and Carbon Nanostructures**

BS/M.Sc students

Sanaa Sharma (B.S.), **Himanshu Kumar** (2 Year M. Sc, 2022 -23), **Chintu Das** (2 Year M. Sc, 2021-22), **Anish Shivamani** (B.S.), **Kailash Sahu** (2 Year M. Sc, 2020-21), **Ravindra Rajpoot** (2 Year M. Sc, 2019-20), **Mahesh Kumar** (2 Year M. Sc, 2018-19), **Subhajit Barman** (2 Year M. Sc, 2018-19), **Valay Agarawal** (B.S.), **Riddhi Ashok Jain** (5 year Int. M. Sc, 2018), **Prasenjit Das** (M. Sc, 2016-18, now: Ph. D. student, Indian Institute of Technology Kharagpur), **Pradeep Billas** (2 Year M. Sc, 2017-18), **Naveen Kumar** (2 Year M. Sc, 2017-18), **Disha Gupta** (5 Year Int. M. Sc, 2017-18), **Vijay Meena** (2 Year M. Sc, 2015-16), **Yash Patel** (5 Year Int. M. Sc, 2015-16), **Tarun Jhunjhunwala** (5 Year Int. M. Sc, 2015-16), **Jayanta Ghosh** (2 Year M. Sc, 2013-14, submitted Ph. D. thesis from Indian Institute of Science Bangalore, now: Post Doc, University of Kassel, Germany), **Himanshu Dixit** (5 Year Int. M. Sc, 2013-14), **Nisheet Patel** (5 Year Int. M. Sc, 2014-15, now: Ph. D. student, University of Geneva), **Shobhit Srivastava** (5 Year Int. M. Sc, 2014-15), **Rahul Biswas** (2 Year M. Sc, 2014-15), **Bibhab Bandhu Majumdar** (M.Sc, 2013-14, completed Ph. D. from the Max Planck Institute for Coal Research, now: Assistant Professor, VIT AP University, Amaravati)

Project assistants/JRF

Minal (SERB sponsored JRF) (June 2023 - December 2023), **Bikramaditya Das** (JRF under SERB project) (August 2022 - April 2023), **Vikarm Gaikwad** (JRF under SERB project) (September 2021 - July 2022), **Sayantani Chakraborty** (JRF under SERB project) (February 2021 - August 2021), **Sk Mujaffar Hussain** (Project Research Assistant, February 2016- April 2016), **Shruti Shriram Jeurkar** (Project Research Assistant, September 2015 - January 2016), **Manuja Kothiyal** (Project Research Assistant, July 2015- September 2015)

Summer/Winter project students

Rohit Raj, Indian Institute of Science, Bengaluru (NIUS Summer Student, June 2020 -), **Santosh Kumari**, Central University of Rajasthan (IAS Summer student, August 2020 -), **Shashank Krishna**, Bharatidashan University (NIUS Summer Student, June 2019 - July 2019), **Divy Gupta**, NISER (Inspire Summer Fellow, May 2019 - July 2019), **Anirudh C S**, MES College, Bangalore (IAS Summer Fellow, June 2018 - August 2018), **Ajesh Saviour Paravila**, NIT Rourkela (NIUS Summer Student, May 2018 - July 2018), **Chinmaya Kumar Jena**, NISER (IAS Summer Fellow, May 2018 - June 2018), **Arya Karumanthra**, Indian Institute of Science Bangalore (Inspire Winter Fellow, December 2017 - January 2018), **Gaurav Mitra**, IIT Kanpur (IAS Summer Fellow, May 2017 - July 2017, now: Ph. D. student, New York University), **Aditya Sarma Phukon**, University of Hyderabad (NIUS Summer Student, June 2017 - July 2017, November 2017 - December 2017, June 2018 - July 2018), now: Ph. D. student, University of Wisconsin-Madison, **Anand C P, Madras**, Christian College (NIUS Winter/Summer Student, May - July 2016, December 2016 - January 2017, May -June 2017), **Mousumi Baruah**, North Eastern Hill University, Shillong (Inspire Winter Fellow, December 2016 - January 2017), **Souvik Dey**, Vishya Bharati (Inspire Summer Fellow, May-July 2016, now: Ph. D. student, University of Illinois at Chicago), **Mahendra Patel**, IISER Pune (Inspire Summer Fellow, May-July 2016), now: Ph. D. student, EPFL, Switzerland, **Arindam Debnath**, St. Stephen's, New Delhi (IAS Summer Fellow, May-July 2016), **Tousif Islam**, IISER Kolkata (Inspire Summer Fellow, May-July 2015), **Rohit Goswami**, HBTI Kanpur (May-July 2015), now; Ph. D. student, University of Iceland, **Punit Kumar Jha**, NISER (Inspire Summer Fellow, May-July 2014, now: Ph. D. student, University of Illinois at Urbana Champaign), **Prachi Sharma**, NISER (Inspire Summer Fellow, May-July 2013, now: Ph. D. student, University of Minnesota), **Manjunath G J**, RIE (NCERT), Mysore (IAS Summer Fellow, May-July

2013, now: Ph. D. student, IST, Austria)

References

- **K. L. Sebastian**

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  Theoretical Physics Institute for Physics and Astronomy — *Voice:* +49 331 977 5985
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- **Arun Yethiraj**

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  Madison, WI 53706
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- **M. Muthukumar**

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- **Swapan Kumar Ghosh**

Distinguished Professor
UM-DAE Centre for Excellence in Basic Sciences — *Voice:* +91-22-26532132
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- **Deb Shankar Ray**

Senior Professor
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Sponsored Research Projects as PI

- **Salary/stipend of graduate students come from other sources, not included in grants.**

- Theoretical investigation of single particle dynamics in condensed phase: Effect of crowding and fluctuation, IRCC, IIT Bombay, 25 Lakhs (30000 US $) (completed).
- Loop formation involving long chain molecules: Effect of viscoelastic solvent, hydrodynamics and chain stiffness, CSIR, 6 Lakhs (7200 US $) (completed).
- Theoretical investigation of the dynamics of tracer molecules in crowded environment and its relevance in cell biophysics, SERB, 30 Lakhs (360000 US $) (completed).
- Theory and simulation of active colloids, IRCC, IIT Bombay 5 Lakhs (6000 US $) (completed).
- Effect of crosslinking agents on the conformational landscape of peptides and its impact on the efficiency of peptide therapeutic, SERB, 43 Lakhs (520000 US $)(completed).
- Wet and Dry Internal Friction in the context of Polymer Dynamics, Matrics SERB, 6 Lakhs (7200 US $) (completed).

Referee/Reviewer Activities

- Journals: *J. Chem. Phys., Biophys. J, Soft Matter, Soft Materials, Phys. Chem. Chem. Phys., J. Phys. A: Math and Theo, Physica A, Chem. Phys. lett., Chem. Phys. Impact, New J. Phys., J. Phys. Chem., ACS Appl. Mat. Int., Small, Proce. Natl. Acad. Sci.(Phys. Sci.) (NASA), J. Chem., J. Theor. Comput. Chem., Eng. Appll. Comput. Flu. Mech., J. Chem. Sci., Int. J. Mod. Phys. B, J. Mol. Model., Euro. Biophys. J, Euro. Phys. J. E, Appl. Math. Model, Front. Phys., Int. J. Non. Lin. Mech., Bull. Mat. Sci., Mol. Simul., J. Chem. Theo. Comput., J. Biomol. Struct. Dyn., Scientific Reports., Comput. Strut. Biotech. J., J. Mol. Liquids, Macromolecules, J. Stat. Mech., Plos Comput. Biol., Langmuir*

  Ph. D. theses from several Institutes, project proposals from SERB (Science and Engineering Research Board) India, NSM (National Supercomputing Mission).

Institute and Departmental activities

- Member, Department policy committee (**DPC**), October 2023 -.
- Faculty Advisor from the Department of Chemistry for SC/ST students, 2022-.
- Member, Undergraduate Performance Evaluation Committee (**UGAPEC**), 2018-2020.
- Associate Warden, Hostel 14, June 2017 - January 2020.
- Faculty Advisor, fifth year Integrated M. Sc and second year 2 year M. Sc in Chemistry, 2013-2018.
- Member, Department policy committee (**DPC**), July 2018 - July 2021.
- Secretary, Department undergraduate committee (**DUGC**), January 2014 - January 2017.
- Former Member, Department webpage and Brochure committee.
- Former-Secretary, Department Faculty search committee.
- Former Member, Department Safety committee.
- Former Member, Digitization and Archiving committee.

Community Service and other activities

- Participation in School-Teacher training program of K. V. School.
- UGC Nominee for K. P. B. Hinduja College of Commerce, Mumbai (Autonomous).

Conferences Organized

- Part of the organizing committee for the In House Symposium, Department of Chemistry, IIT Bombay, 2 March 2013.
- Part of the organizing committee for the 16th CRSI National Symposium in Chemistry and 8th CRSI-RSC Joint Symposium in Chemistry, 6-9 February 2014, IIT Bombay.
- Convener for the conference, Physical and Biophysical Chemistry: Theory and Experiment, 4-6 December, 2015, IIT Bombay.
- One of the organizers for the meeting, Soft Matter and Statistical Mechanics 2019, 4-5 January, 2019, IISER Pune.
- Part of the organizing committee for the meeting Ultrafast Sciences 2019, 7-9 November, IIT Bombay.
- Part of the local organizing committee for CompFlu 2020, 10-12 December, IIT Bombay.
- Convenor: Physical Chemistry Physical Biology 2021, 24-28 September 2021, Virtual Platform.
- Convenor: Joint Chemistry and Chemical Engineering Soft Matter and Biophysics Meeting, 23 June, 2022, IIT Bombay.
- Convenor: Mini Meeting on Statistical Mechanics, Soft and Living Matter, 10 March, 2023. IIT Bombay.
- Convenor: Mini-Symposium on Theoretical Physical Chemistry and Chemical Physics (MS-TPCCP), 28-29 July, 2023, IIT Bombay.
- One of the organizers: Symposium on Soft and Biological Materials: Experiments and Theory, 14 December 2023, IIT Bombay.
- Convenor: Theoretical Chemistry Symposium (TCS), Indian Institute of Technology Bombay, December 2025.