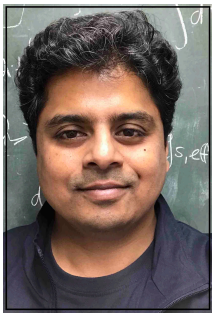

Arnab Bhattacherjee

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School of Computational & Integrative Sciences,
Jawaharlal Nehru University
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RESEARCH VISION & ACADEMIC LEADERSHIP

I lead a research group at the interface of theoretical biophysics, molecular simulations, and genome biology, focusing on the physical principles underlying chromatin organization and gene regulation. My group develops multiscale physical and AI-integrated models that connect Hi-C/Micro-C data with nucleosome dynamics and protein–DNA interactions. This work has resulted in a sustained body of peer-reviewed publications, the training of doctoral researchers who have progressed to faculty and postdoctoral positions abroad, and continuous national and international research support.

PROFESSIONAL PROFILE

- Associate Professor, School of Computational and Integrative Sciences, Jawaharlal Nehru University, India

WORK HISTORY

Associate Professor, 2020 - till date
School of Computational and Integrative Sciences,
Jawaharlal Nehru University

Assistant Professor, 2015 - 2020
School of Computational and Integrative Sciences,
Jawaharlal Nehru University

Assistant Professor & 2014 - 2015
DST Inspire Faculty, IIIT Delhi, India

Post Doctoral Fellow, 2013 - 2014
Weizmann Institute of Science, Israel

Post Doctoral Fellow, 2011 - 2013
Theoretical Physics Division,
Lund University, Sweden

EDUCATION

Doctor of Philosophy in Science 2010
Department of Chemistry,
University of Delhi, India
Supervisor: Prof. Parbati Biswas.
Statistical Theory of Designing Evolutionary Fit Protein Sequences.

Examiners: Prof. Deb Shankar Ray (IACS), Prof. Anil Kumar(NCL Pune), Prof. Amalendu Chandra (IIT Kanpur)

Master in Science 2006
Physical Chemistry Specialisation
Ranked First in the College
Department of Chemistry,
University of Delhi, India

Bachelor in Science 2004
Chemistry Honours
St. Xavier's College, Calcutta
University of Calcutta, India

RESEARCH INTERESTS

Research Vision: Deciphering the physical principles governing genome organization and gene regulation using multiscale computational modeling, with a focus on mechanisms underlying genomic diseases and developmental defects.

- **3D Genome Architecture & Chromatin Dynamics:** Elucidating high-resolution genome organization using experimentally informed polymer models; investigating nucleosome breathing dynamics and the invasion mechanisms of pioneer transcription factors.
- **Protein-DNA Recognition Kinetics:** Unraveling the mechanisms of facilitated diffusion and target search in crowded intracellular environments ; analyzing the role of DNA shape deformation and topology in transcription factor binding specificity.
- **Intrinsically Disordered Proteins (IDPs):** Modeling the conformational dynamics and aggregation pathways of disease-linked IDPs, focusing on inter-domain crosstalk and phase separation drivers.
- **Methodological Development:** Development of GPU-accelerated coarse-grained models, enhanced sampling algorithms, and effective force fields to bridge the gap between theoretical biophysics and experimental observations.

AWARDS/HONOURS/FELLOWSHIPS

- Recipient of CRSI Young Scientist Award in the 30th CRSI-NSC meeting of Chemical Research Society of India, held between 3-5th February 2023.
- Recipient of INSA medal for young scientists 2022, India.
- Recipient of Humboldt Research Fellowship for Experienced Researchers from Alexander von Humboldt Foundation, Germany, 2022.
- Elected Associate of the Indian Academy of Sciences (IASc), August 2020 - December 2023.
- Joined Editorial Board of Biophysics as Review Editor for Frontiers in Physics, Frontiers in Physiology and Frontiers in Molecular Biosciences.
- Indo-U.S. Science and Technology Forum (IUSSTF) Award for supporting Indo-US Symposium on 'Multiscale Simulation and Mathematical Modelling of Complex Biological Systems (WS-61/2018) - January 2019
- Department of Science and Technology SERB Conference Grant (SSY/2018/001225) - December 2018
- Conference Grant from Council of Scientific and Industrial Research (SYM/9982/18-HRD). January 2019.
- Conference Grant from Indian National Science Academy (SP/C-DEC/21/2018/19). January 2019.
- Incentive awards for publications - 2017 by Department of Biotechnology, Government of India.
- Department of Science and Technology INSPIRE Faculty awardee, December 2013.
- Received postdoctoral fellowship from Weizmann Institute of Science, 2013 - 2014
- Received Royal Swedish Physiographic Society postdoctoral fellowship, 2011 - 2013.
- Ranked 9th in All India Lectureship examination(CSIR), 2010.
- Received CSIR Research Fellowship (Senior Research Fellow), 2010 - 2011.

- Received Award for poster presentation in IISc Bangalore at Theoretical Chemistry Symposium, 2009.
- Received DST Research Fellowship (Junior and Senior Research Fellow) 2006 - 2009.
- M.Sc College Topper Scholarship (1st and 2nd year).
- Merit Scholarship (1999) in 10th standard for acquiring a position within first 100 in West Bengal.

RESEARCH PUBLICATIONS IN REVIEWED JOURNALS

(**Summary:** *Nature Communications*: 1, *Nucleic Acids Research*: 4, *Biophysical Journal*: 5, *Journal of Physical Chemistry B*: 7, *JACS Au*: 1, Other journals: *Soft Matter*, *WIREs Computational Molecular Science*, *PLoS Computational Biology*, *Scientific Reports*, *PCCP*, *ChemPhysChem*, *Frontiers Mol. Biosci.*, *Life*, *BBA*, *J. Biochemistry*, *J. Chem. Sci.*, *Phys. Rev. E*) [* corresponding author]

- An Experimentally Informed Polymer Model Reveals High Resolution Organization of Genomic Loci, Rahul Mittal, Dieter Heermann & **Arnab Bhattacherjee***, *Nature Communications* (Accepted), Nov 2025.
- Shape-aware Diffusivity of DNA Binding Proteins Undergoing Rotation-coupled Sliding Dynamics along DNA, Shrawan K Choudhary, Kavana P Keshava, **Arnab Bhattacherjee***, *The Journal of Physical Chemistry B* (Accepted), Nov 2025
- Modeling Facilitated Diffusion of Proteins in Crowded Environment, Shrawan K Choudhary, Sangeeta, Pinki Dey & **Arnab Bhattacherjee***, *Subcell Biochem*. 2025:109:499-529. Springer Nature.
- Role of shape deformation of DNA binding sites in regulating the efficiency and specificity in their recognition by DNA binding proteins, Sangeeta, Sujeet Kumar Mishra, & **Arnab Bhattacherjee***, *Journal of American Chemical Society Au*, 4(7):2640-2655, 2024.
- Nick Induced Dynamics in Supercoiled DNA Facilitates Protein Target Search Process, Sangeeta & **Arnab Bhattacherjee***, *Journal of Physical Chemistry B*, 128(34):8246-8258, 2024.

- The Role of Nucleotide Opening Dynamics in Facilitated Target Search by DNA-Repair Proteins, Sujeet Kumar Mishra, Sangeeta, Dieter W. Heermann & **Arnab Bhattacherjee***, *BBA - Gene Regulatory Mechanisms*, 1867(2):195026, 2024.

- Unusual weak and delayed GTPase activity of FtsZ from human pathogenic bacteria Helicobacter pylori, Sumiran Kumar Gurung, Sangeeta, Priyanka Dubey, Fatima Akhtar, Abhik Saha, **Arnab Bhattacherjee***, Suman Kumar Dhar*., The *Journal of Biochemistry*, 175 (4):405-417, 2024.

- How Do Nucleosome Dynamics Regulate Protein Search on DNA? Sujeet Kumar Mishra and **Arnab Bhattacherjee***, *Journal of Physical Chemistry B,* 127(25), 5702–5717, 2023.

- Understanding the Target Search by Multiple Transcription Factors on Nucleosomal DNA, Sujeet Kumar Mishra and **Arnab Bhattacherjee***, *ChemPhysChem.* 24(8), e202200644. 2023.

- Interdomain crosstalk in human RPA regulates kinetics and thermodynamics of its binding to ssDNA, Sangeeta and **Arnab Bhattacherjee***, *PLOS One*, 18(1): e0278396 2023.

- Torsional behaviour of supercoiled DNA regulates recognition of architectural protein Fis on minicircle DNA, Anupam Mondal, Sangeeta and **Arnab Bhattacherjee***, *Nucleic Acids Research*, 50, 6671-6686, 2022.

- Understanding Protein Diffusion on Force Induced Stretched DNA Conformation, Anupam Mondal, and **Arnab Bhattacherjee***, *Frontiers in Molecular Biosciences*, 9:953689, 2022.

- Nucleosome breathing facilitates cooperative binding of pluripotency factors Sox2 and Oct4 to DNA, Anupam Mondal, Sujeet Kumar Mishra and **Arnab Bhattacherjee***, *Biophysical Journal*, 121(23), 4526-4542, 2022.

- Superstructure Detection in Nucleosome Distribution Shows Common Pattern within a Chromosome and within the Genome, Sujeet Kumar Mishra, Kunhe Li, Simon Brauburger, **Arnab Bhattacherjee**, Nestor Norio Oiwa, and Dieter Heermann, *Life*, 12, 541, 2022.

- Kinetic Origin of Nucleosome Invasion by Pioneer Transcription Factors, Anupam Mondal, Sujeet Mishra and **Arnab Bhattacherjee***, *Biophysical Journal*,**120**, 5219-5230, 2021.

- Mechanism of Dynamic Binding of Replication Protein A to ssDNA, Anupam Mondal and **Arnab Bhattacherjee***, *Journal of Chemical Information and Modelling.* **60,** 5057-5069, 2020.

- BCG Vaccination Policy and Preventive Chloroquine Usage: Do They Have an Impact on COVID-19 Pandemic?, Abhibhav Sharma, Saurabh Kumar Sharma, Yufang Shi, Gerry Melino, **Arnab Bhattacherjee*** and Gobardhan Das, *Nature Cell Death and Disease*. **11,** 516, 2020.

- Molecular Dynamics Simulations and Biochemical Characterization of Pf14-3-3 and PfCDPK1 Interaction Towards its Role in Growth of Human Malaria Parasite. Ravi Jain, Pinki Dey, Sakshi Gupta, Soumya Pati, **Arnab Bhattacherjee**, Manoj Munde, and Shailja Singh. *Biochemical Journal*, 477(12):2153-2177, 2020.

- Structural Basis of Enhanced Facilitated Diffusion of DNA Binding Proteins in Crowded Cellular Milieu. Pinki Dey and **Arnab Bhattacherjee***
  Biophysical Journal. 118(2):505-517, 2020

- Facilitated Diffusion of DNA Repair Proteins in Crowded Cellular Environment - A Case Study with Human Uracil DNA Glycosylase. Pinky Dey and **Arnab Bhattacherjee*** *Journal of Physical Chemistry B.* 123(49):10354-10364, 2019

- Disparity in Anomalous Diffusion of Proteins Searching for their Target DNA Sites in a Crowded Medium is Controlled by Size, Shape and Mobility of Macromolecular Crowders. Pinki Dey and **Arnab Bhattacherjee*,** *Soft Matter.* 15, 1960, 2019. The research is highlighted as Cover Page image of the journal.

- Role of Macromolecular Crowding on the Intracellular Diffusion of DNA Binding Proteins. Pinki Dey and **Arnab Bhattacherjee***, *Scientific Reports.* 8, 844, 2018.

- Understanding the Role of DNA Topology in Target Search Dynamics of Proteins. Anupam Mondal and **Arnab Bhattacherjee***, *Journal of Physical Chemistry B.* 12, 9372-9381, 2017.

- Coarse-grained models for studying protein diffusion along DNA. **Arnab Bhattacherjee***, Dana Krepel and Yaakov Levy. *WIREs Computational Molecular Science.* 6, 515, 2016.

- Searching target sites on DNA by proteins: Role of DNA dynamics under confinement. Anupam Mondal and **Arnab Bhattacherjee***. *Nucleic Acids Research.* 43, 9176–9186, 2015.

- Thermodynamic Protein Destabilization by GFP Tagging: A Case of Interdomain Allostery. Miri Sokolovski, **Arnab Bhattacherjee**, Naama Kessler, Yaakov Levy, Amnon Horovitz. *Biophysical Journal*, 109(6), 1157-1162, 2015.

- Search by proteins for their DNA target site: 2. The effect of DNA conformation on the dynamics of multidomain proteins. **Arnab Bhattacherjee** and Yaakov Levy. *Nucleic Acid Research*, 42(20), 12415, 2014.

- Search by proteins for their DNA target site: 1. The effect of DNA conformation on protein sliding. **Arnab Bhattacherjee** and Yaakov Levy. *Nucleic Acid Research*, 42(20), 12404, 2014.

- Conformational properties and aggregation of the 1-93 fragment of apolipoprotein A-I. Jitka Petrlova, **Arnab Bhattacherjee**, Wouter Boomsma, Stefan Wallin, Jens Lagerstedt and Anders Irbäck. *Protein Science* 23(11), 1559, *2014*.

- Hybrid Monte Carlo with Non-Uniform Step Size. Christian Holzgräfe, **Arnab Bhattacherjee** and Anders Irbäck. *Journal of Chemical Physics*. 140, 044105, 2014.

- Exploring protein-peptide binding specificity through computational peptide screening. **Arnab Bhattacherjee** and Stefan Wallin. *PLOS Computational Biology* 9 (10), e1003277, 2013.

- Coupled Folding-Binding in a Hydrophobic/Polar Protein Model: Impact of Synergistic Folding and Disordered Flanks. **Arnab Bhattacherjee** and Stefan Wallin. *Biophysical Journal*. 102, 569, 2012.

- Role of Conformational Heterogeneity on Protein Misfolding. Anupaul Baruah, **Arnab Bhattacherjee** and Parbati Biswas. *Soft Matter* 8 (16), 4432, 2012.

- Designing Misfolded Protein Sequences by Energy Landscaping. **Arnab Bhattacherjee** and Parbati Biswas. *Journal of Physical Chemistry B*. 115 (1), 113, 2011.

- Role of Foldability and Stability in Designing Real Protein Sequences. **Arnab Bhattacherjee** and Parbati Biswas. *Physical Chemistry Chemical Physics*. 13, 9223, 2011. Selected in the list of Top 20 Articles, in the Domain of Article 21468433, Since its Publication (2011).

- Neutrality and Evolvability of Designed Protein Sequences. **Arnab Bhattacherjee** and Parbati Biswas. *Physical Review E*. 82, 011906, 2010. Also selected for 15th July 2010 issue of Virtual Journal of Biological Physics Research.

- Statistical Theory of Neutral Protein Evolution by Random Site Mutations. **Arnab Bhattacherjee** and Parbati Biswas. *Journal of Chemical Sciences*. 121 (5), 887, 2009.

- Combinatorial Design of Protein Sequences with Application to Lattice and Real Proteins. **Arnab Bhattacherjee** and Parbati Biswas. *Journal of Chemical Physics*. 131, 125101, 2009. Also selected for 1st October 2009 issue of Virtual Journal of Biological Physics Research.

- Statistical Theory of Protein Sequence Design by Random Mutation. **Arnab Bhattacherjee** and Parbati Biswas. *Journal of Physical Chemistry B*. 113 (16), 5520, 2009.

RESEARCH PROJECTS (TOTAL FUND SECURED: 2.26 CR)

Ongoing:

- DST SERB sponsored project titled *Understanding the structure function relationship of eukaryotic genome through a multiscale approach* (CRG/2023/000636). - approved (~ 61.74 Lacs)

- DBT India sponsored project titled *Unravelling the molecular basis of protein-ssDNA interactions through a combined computational and experimental approaches* (BT/PR46267/BID/7/1015/2023). - approved (~ 42.12 Lacs)

Completed:

- DST SERB sponsored project titled *Invading Nucleosome: Understanding How Cells Recruit Proteins at Target DNA Sites* (CRG/2019/001001). - Completed (~ 40 Lacs)

- Study of searching mechanism of DNA binding proteins on nucleosome using a mathematical model and stochastic simulation, MATRICS, DST Ongoing (~ 06 Lacs)

- DST INSPIRE project titled *Understanding the role of DNA flexibility in Protein-DNA recognition* (DST/INSPIRE/04/2013/000100) - Completed (35 Lacs)

- DST SERB sponsored project titled *Positive and negative impacts of macro molecular crowding during target site location by DNA binding proteins-origin of optimal search at physiological ionic concentration* (ECR/2016/000188). - Completed. (30 Lacs)

- UPOE-II project titled *Engineering DNA binding proteins by modulating dynamic conformational ensemble of proteins and DNA flexibility*, project id 259. - Completed (11 Lacs)

International Support:

- Humboldt Fellowship (Experienced Researcher)

- IUSSTF Symposium Grant

INVITED LECTURES (LAST FIVE YEARS)

- *Understanding Protein-DNA Recognition Across Scales,* TCS-2025, December 2025, IIT Bombay.

- *From Diffusion to Decision,* IACS, October 2025.

- *Uncovering High-Resolution Organization of Genomic Loci using Experimentally Informed Polymer Model,* PHYSICAL CHEMISTRY SYMPOSIUM, IIT Patna October 2025.

- *Uncovering High-Resolution Organization of Genomic Loci using Experimentally Informed Polymer Model*, Recent Trends in Biophysics and Spintronics meeting 2025, Ashoka University, March 10-12, 2025.

- *Uncovering High-Resolution Organization of Genomic Loci using Experimentally Informed Polymer Model*, Annual Meeting of Indian Biophysical Society, IIT Madras, March 06-09, 2025.

- *Uncovering High-Resolution Organization of Genomic Loci using Experimentally Informed Polymer Model*, Horizons in Structural and Computational Biology 2025, IIT Hyderabad, February 28 - March 01, 2025.

- *Uncovering High-Resolution Organization of Genomic Loci using Experimentally Informed Polymer Model,* Physics and Chemistry of Atomic, Molecular and Condensed Matter Systems (PCAMC-2024), IISER Kolkata, December 11-14, 2024.

- *Uncovering High-Resolution Organization of Genomic Loci using Experimentally Informed Polymer Model,* Physics and Chemistry of Atomic, Molecular and Condensed Matter Systems (PCAMC-2024), IISER Kolkata, December 11-14, 2024.

- Role of Shape Deformation of DNA-Binding Sites in Regulating the Efficiency in Their Recognition by DNA-Binding Proteins, PHYSICAL CHEMISTRY SYMPOSIUM, IIT Bombay October 2024.

- *Mechanism of Reading DNA,* Regional Young Investigator Meeting (RYIM), IBITS Pilani, January 2024.

- Decoding the sequence binding specificity in indirect-DNA readout mechanism, PHYSICAL CHEMISTRY SYMPOSIUM, IIT Kanpur October 2023.

- *Understanding protein diffusion on DNA using coarse-grained models,* Heidelberg Institute for Theoretical Studies, Germany, August 2023.

- *Nuclear Traffic and Transport: Rule of Faster Protein Communication on DNA,* Statistical Mechanics in Chemistry and Biology (SMCB) seminar series, March 2023.

- *Molecular Simulations: Watching biomolecules at work using computers,* Summer Undergraduate Research Programme (SURP), ACBR, Delhi University June 2023.

- *Decoding the sequence binding specificity in indirect-DNA readout mechanism,* PHYSICAL CHEMISTRY SYMPOSIUM, IIT Kanpur October 2023.

- *Nuclear Traffic and Transport: How proteins search their target sites?* Stochastic Biological Physics, ICTS, Bangalore October 2022.

- *Understanding Chemistry between ssDNA and Replication Protein A*, International Conference on Physical Chemistry and Physical Biology, 27th September 2021.

- *Nuclear Traffic and Transport: Rule of Faster Protein Communication*, Theoretical Chemistry Symposium, 14th December 2021.

- *How Proteins Travel on DNA Tracks*, International Conference on "RECENT ADVANCES IN BIOTECHNOLOGY, BIOINFORMATICS & BIOCHEMISTRY, 20th December 2020.

- *How Proteins Travel on DNA Tracks*, ICTS-"Statistical Biological Physics: From Single Molecule to Cell (ONLINE)" 8th December 2020

- *Understanding Protein Transport on DNA Track*, Annual Meeting of Indian Academy of Sciences 8th November 2020.

PRESENTATIONS IN CONFERENCE/SYMPOSIUM/WORKSHOP BY PHD STUDENTS (FROM JNU)

(International Travel grant: 3, Oral Presentation award: 2, Best poster awards: 4)

- Poster Presentation: "From Contacts to Patterns: Quantifying Structural Changes in Hi-C Data" at the 47th Indian Biophysical Society (IBS) Meeting, IIT Madras, Chennai (6–9 March 2025). Best Poster Award – Kavana Priyadarshini K.

- Poster Presentation: "Uncovering High-Resolution Organization of Genomic Loci using an Experimentally Informed Polymer Model" at the Conference on Advances in Molecular and Cellular Biology, Convention Centre, JNU, New Delhi (2 December 2025). Rahul Mittal.

- Poster Presentation: "Uncovering High-Resolution Organization of Genomic Loci via Multiscale Polymer Simulations" at SoPhyC-2024, IIT Bombay (22–25 October 2024). Rahul Mittal.

- Short Talk: "A Physical Model to Understand the High-Resolution Chromosome Organization in Interphase" at the symposium "Simulations of Physical and Biological Systems", JNU, New Delhi (1 March 2024). Rahul Mittal.

- Poster Presentation: "How Transcription Factors Recognize Target Sites on DNA through DNA Shape Information" at the JNCASR–CECAM Conference MD@60 (26–29 February 2024). Shrawan Kumar Choudhary.

- Poster Presentation: at the IUPAB Congress 2024, Kyoto International Conference Centre, Kyoto, Japan (June 2024). Sangeeta

- Presentation: Scientegration-2023, School of Computational & Integrative Sciences, JNU, New Delhi (19–20 October 2023). Kavana Priyadarshini K.; Shrawan Kumar Choudhary.

- Presentation: Scientegration-2023 – Best Oral Presentation Award. Sangeeta

- Oral Presentation: 4th Annual Ph.D. Symposium, School of Computational & Integrative Sciences, JNU, New Delhi (October 2023). Sangeeta

- Poster Presentation: SoPhyC-2023 – Physical Chemistry Symposium, IIT Kanpur (October 2023). Sangeeta

- Presentation: Scientegration-2023, School of Computational & Integrative Sciences, JNU, New Delhi. Anupam Mondal.

- Short Talk: “A GPU-based Physical Model to Understand the High-Resolution Genome Organization and Function” at the ICTS Program: Statistical Biological Physics – From Single Molecule to Cell, ICTS-TIFR, Bengaluru (11–22 October 2022). Rahul Mittal.
- Short Talk: at the ICTS Program: Statistical Biological Physics – From Single Molecule to Cell, ICTS-TIFR, Bengaluru (October 2022). Kavana Priyadarshini K.; Sangeeta.
- Flash Talk & Poster Presentation: EMBO Lecture Course on Functional Nucleic Acids, Regional Centre of Biotechnology, Faridabad (August 2022). Sangeeta.
- E-Poster Presentation: IBS-2022 – Conceptual Advances in Biophysics and its Applications, ACTREC, Tata Memorial Centre, Navi Mumbai (March 2022). Sangeeta.
- Poster Presentation: Protein–DNA Interactions: From Biophysics to Cell Biology, Weizmann Institute of Science, Israel. Sujeet Kumar Mishra.
- Paper Presentation & Best Oral Presentation Award: Scientegration-2022, School of Computational & Integrative Sciences, JNU, New Delhi. Sujeet Kumar Mishra.
- Oral Presentation: PCPB-2021 – Physical Chemistry & Physical Biology Conference. Anupam Mondal
- Participation: SMCB-2021 – Statistical Mechanics in Chemistry and Biology Conference. Sujeet Kumar Mishra; Sangeeta
- Participation: MSMM-2021 (Online) – Multiscale Simulation & Mathematical Modelling of Complex Biological Systems, JNU, New Delhi. Rahul Mittal; Anupam Mondal; Sujeet Kumar Mishra; Sangeeta.
- Oral Presentation: Albany-2019: The 20th Conversation (International Conference). Anupam Mondal.
- Poster Presentation: MSMM-2019 – Multiscale Simulation & Mathematical Modelling of Complex Biological Systems. Anupam Mondal.
- Poster Presentation & Best Poster Prize (Ratna Phadke Award): Annual Symposium of the Indian Biophysical Society, IISER Mohali. Anupam Mondal.
- Poster Presentation: 17th International Conference on Bioinformatics (INCOB). Anupam Mondal.
- Workshop Participation: INCOB-2018 Workshop on Programmatic Access to Protein Sequence, Function and Structure (UniProt & PDBe), JNU, New Delhi. Sujeet Kumar Mishra.

REVIEWER ASSIGNMENT

- Advanced Science
- Nucleic Acids Research
- Journal of Physical Chemistry Letters
- Journal of Physical Chemistry B

- Biophysical Journal
- PLOS One
- Protein Science
- Soft Matter
- Polymers
- BMJ Open
- BMC Medical Genomics
- Scientific Reports
- Physical Chemistry Chemical Physics
- Journal of Biomolecular Structure and Dynamics.

SUPERVISION

PHD

- **Sangeeta**
  Thesis Title:. *Understanding the Transport of Proteins on DNA Track using in Silico Modelling.* Sangeeta has been awarded the prestigious Prime Minister's Research Fellowship (PMRF). **Year of Award: 2025**.

- **Sujeet Kumar Mishra**
  Thesis Title: *Diffusion of Proteins on DNA - Role of Genome Organisation and its Structural Dynamics.* Sujeet is also selected for a dual PhD program with Heidelberg university, Germany. **Year of Award: 2024**

- **Anupam Mondal**
  Thesis Title: *Understanding the Role of Structural and Functional Dynamics of DNA in Protein-DNA Recognition Using Theoretical and Computational Approaches.* **Year of Award: 2022**

- **Pinki Dey**
  Thesis Title: *Understanding the Role of Macromolecular Crowding on Target Search Dynamics of DNA Binding Proteins.* **Year of Award: 2019**

PHD(ONGOING)

- Supervising Rahul Mittal (M.Sc Physics, IIT Mandi)
- Supervising Kavana Priyadarshi K (M.Sc in CompBio, SCIS).
- Supervising Shrawan Chaudhury (M.Sc Biotechnology, IIT Bombay).
- Gargi Gautam (M.Sc Microbiology, Central University of Rajasthan)

POSITIONS HELD BY FORMER PHD AND POSTDOC STUDENTS

- **Pinki Dey**
  2025-Present: Faculty, Torrens University, Australia.

- **Anupam Mondal**
  2025-Present: Postdoctoral Fellow, Texas A&M University, Texas, USA, Advisor:

Prof. Jeetain Mittal.
2022-2025: Postdoctoral Fellow, Center for Theoretical Biological Physics (CTBP) and Department of Chemistry, Rice University, Houston, Texas, United States, Advisor: Prof. Anatoly Kolomeisky.

- **Sujeet Kumar Mishra**
  2024-Present: Department of Chemical & Structural Biology, Postdoctoral Fellow (Molecular Systems Biophysics). Advisor: Prof. Hagen Hofmann

- **Sangeeta**
  2025-present: Faculty, Hindu College, Delhi University.

- **Pravin Kumar**
  Assistant Professor, UPES, Dehradun, India

MASTER/PROJECT STUDENTS

- **Souraj Das**
  M.Sc. Dissertation (2024-2025), School of Computational & Integrative Sciences, JNU

- **Trisha Majumdar**
  M.Sc. Dissertation (2024-2025), School of Computational & Integrative Sciences, JNU

- **Vikash Mahato**
  PGD Dissertation (2024-2025), School of Computational & Integrative Sciences, JNU

- **Kaushal Grover**
  M.Sc. Dissertation (2023-2024), School of Computational & Integrative Sciences, JNU

- **Tarun**
  M.Sc. Dissertation (2022-2023), School of Computational & Integrative Sciences, JNU

- **Marvin Prakash**
  MS Dissertation (2022-2023), School of Computational & Integrative Sciences, JNU

- **Shidharth Anand**
  MS Dissertation (2022-2023), School of Computational & Integrative Sciences, JNU

- **Alok Anand**
  M.Sc. Dissertation (2020-2021), Present position - Ph.D. student, IIIT Delhi, New Delhi, India

- **Ashik Babu P**
  M.Sc. Dissertation (2020-2021), Present position - Ph.D. student, SC&IS, JNU, New Delhi, India

- **Subhankar Sarkar**
  M.Sc. Dissertation (2020-2021), Present position - Ph.D. student, IIT Delhi, New Delhi, India

- **Sujeet Kumar Mishra**
  M.Sc. Dissertation (2017-2018), Present position - Postdoctoral Fellow with Prof. Hagen Hofmann Weizmann Institute of Science, Rehovot, Israel

- **Sautik Samui**
  PGD Dissertation (2021-2022), School of Computational & Integrative Sciences, JNU

- **Nitin Chaturvedi**
  PGD Dissertation (2021-2022), School of Computational & Integrative Sciences, JNU

- **Anushna Bhattacharjee**
  Project Student (March - July 2025)

- **Debarshi Bose**
  Project Student (Indian Academy of Sciences) (June-July, 2024), Present position - B.Sc. student, Presidency University, Kolkata, West Bengal, India

- **Ronak Dsouza**
  Project Student (Indian Academy of Sciences) (April-May, 2024)
  Present position - B. Pharmacy student, Kle College of Pharmacy Belgaavi, Karnataka, India

- **S. Aswathi**
  Project Student (Indian Academy of Sciences) (July-August, 2023), Present position - M.Sc. student Amrita Vishwa Vidyapeetham, Coimbatore, India

- **Afrin Riaz**
  Project Student (July, 2023), Present position - BS-MS Dual Degree, IISER Kolkata, Kolkata, India

- **Manas Joshi**
  Project Student (Indian Academy of Sciences) (July-August, 2021) Present position - Ph.D. student, Boston College, Massachusetts, USA

- **Shiv Rekhi**
  Project Student (June-July, 2020), Present position - Ph.D. student, Texas A&M University, Texas, USA

- **Sangeeta**
  Project Student (2018 - 2019), Research Topic: Protein-DNA Interaction

- **Dr. Venkataramana Inamdi**
  Postdoctoral Fellow (2018 - 2019), Present position - Indian Institute of Technology (IIT), Madras

- **Sakshi Khawal**
  Project student (2016 summer)
  Research Topic: Role of DNA sequence dependent conformational dynamics on target search mechanism of DNA binding proteins, Present position - Ph.D student in University of Côte d'Azur

- **Prasant Chidelia**
  Project student (IITD, 2015 - 2016), Research Topic: Developing GPU based Biosimulator for Nucleic Acids Present position - Working in Microsoft

TEACHING

Jawaharlal Nehru University (JNU), School of Computational and Integrative Sciences

- **Statistical Mechanics of Complex Systems** (M.Sc.; ~20 hours)
  Coverage includes ensembles, stochastic processes, entropy, phase transitions, and applications to biological and soft-matter systems.

- **Statistical Mechanics of Biomolecules and Simulations** (M.Sc./PhD.; ~40 hours)
  Focus on molecular dynamics, Monte Carlo methods, force fields, sampling techniques, thermodynamic integration, and free-energy calculations.

- **Computational and Structural Biology** (M.Sc.; ~20 hours)
  Structure–function relationships of biomolecules, protein folding, molecular recognition, and computational modeling tools.

- **Thermodynamics and Kinetics** (M.Sc.; ~13 hours)
  Classical and nonequilibrium thermodynamics, chemical kinetics, transition-state theory, and biological rate processes.

- **Numerical Techniques and Simulations** (M.Sc.; ~40 hours)
  Numerical integration schemes, random number generation, sampling algorithms, error analysis, and large-scale scientific simulations.

- **Fundamentals of Data Structures and Computer Programming** (M.Sc.; ~40 hours) Algorithms, data structures, and scientific programming with applications in computational physics and biology.

- **Advanced Topics in Physical Sciences** (M.Sc.; ~40 hours)
  Research-oriented course covering contemporary topics in theoretical and computational biophysics.

Indraprastha Institute of Information Technology Delhi (IIIT-Delhi)

- **Molecular Mechanics and Biological Physics** (M.Sc./Ph.D.; ~40 hours)
  Principles of molecular mechanics, coarse-grained modeling, biomolecular simulations, and applications to biological systems.

- **Biophysics** (M.Sc.; ~40 hours)
  Physical principles underlying biological organization, biomolecular interactions, and thermodynamics of living systems.

ACADEMIC SERVICES:

- Convenor of hands on workshop of Macromolecular Structure Solution and Refinement (speaker: Prof. Stefan Knight, Uppsala University), 18-20th March 2025.

- Convenor of one-day symposium on "Simulations of Physical and Biological Systems" held on 1st March 2024 at JNU, New Delhi.

- Member of Local Organising Committee of "30th CRSI National Symposium in Chemistry and 16th CRSI RSC Joint Symposium" Organized by Jawaharlal Nehru University to be held during 2 5 February, 2023.

- Convenor. International conference-cum-workshop on "Multiscale Simulations and Mathematical Modelling of Complex Biological Systems" in Jawaharlal Nehru University, New Delhi, March 01- 06, 2021.

- Convenor. International conference-cum-workshop on "Multiscale Simulations and Mathematical Modelling of Complex Biological Systems" in Jawaharlal Nehru University, New Delhi, January 28 - February 01, 2019.

- Organiser. Conference on "NanoBio Interface" in School of Computational and Integrative Sciences and School of Biotechnology, Jawaharlal Nehru University, New Delhi, March 18-20, 2016,

- Coordinator. A four-week orientation program for faculty at the Human Resource Development Center, Jawaharlal Nehru University, New Delhi, 3rd October 2nd November.

COURSES ATTENDED

- UGC sponsored Orientation course at Human Resource Development Centre, Jawaharlal Nehru University, 2016.
- UGC sponsored Refresher course at Human Resource Development Centre, Jawaharlal Nehru University, 2017.

REFERENCES

Available upon request.