



Arnab Bhattacharjee

Office No: 35, Ground Floor,
School of Computational & Integrative Sciences,
Jawaharlal Nehru University
New Delhi-110067
arnab@jnu.ac.in
URL: <http://ccbb.jnu.ac.in/arnab/>

PROFESSIONAL PROFILE

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

WORK HISTORY

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| Associate Professor, School of Computational and Integrative Sciences, Jawaharlal Nehru University | 2020 - till date |
| Assistant Professor, School of Computational and Integrative Sciences, Jawaharlal Nehru University | 2015 - 2020 |
| Assistant Professor & DST Inspire Faculty, IIT Delhi, India | 2014 - 2015 |
| Post Doctoral Fellow, Weizmann Institute of Science, Israel | 2013 - 2014 |
| Post Doctoral Fellow, Theoretical Physics Division, Lund University, Sweden | 2011 - 2013 |

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

Broad Area: Understanding genome biophysics and its structure-function relationship that has long-term implications for combating medical conditions including cancer and developmental defects by using **computational biology** techniques and **theoretical biophysics principles**. Current research interests include:

- Genome organisation and function - Recognition of causal genes for genomic diseases and developmental defects
- Nucleosome biophysics.
- Diffusion of molecular motors on biological track.
- Probing transcription factor kinetics under various cellular condition.
- Dynamics of disease-linked Intrinsically Disordered Proteins (IDPs) and their aggregation mechanisms.
- Multiscale Simulations, Sampling algorithms and Effective force field Development.

AWARDS/HONOURS/FELLOWSHIPS

- Recipient of prestigious INSA medal for young scientists 2022, India.
- Recipient of prestigious 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

1. Understanding the Target Search by Multiple Transcription Factors on Nucleosomal DNA, Sujeet Kumar Mishra and **Arnab Bhattacharjee**, *ChemPhysChem*. <https://doi.org/10.1002/cphc.202200644>. 2023.
2. Interdomain crosstalk in human RPA regulates kinetics and thermodynamics of its binding to ssDNA, Sangeeta and **Arnab Bhattacharjee**, *Plos One*, 18(1): e0278396 2023.
3. Torsional behaviour of supercoiled DNA regulates recognition of architectural protein Fis on minicircle DNA, Anupam Mondal, Sangeeta and **Arnab Bhattacharjee**, *Nucleic Acids Research*, 50, 6671-6686, 2022.
4. Understanding Protein Diffusion on Force Induced Stretched DNA Conformation, Anupam Mondal, and **Arnab Bhattacharjee**, *Frontiers in Molecular Biosciences*, 9:953689, 2022.
5. Nucleosome breathing facilitates cooperative binding of pluripotency factors Sox2 and Oct4 to DNA, Anupam Mondal, Sujeet Kumar Mishra and **Arnab Bhattacharjee**, *Biophysical Journal*, 121(23), 4526-4542, 2022.
6. Superstructure Detection in Nucleosome Distribution Shows Common Pattern within a Chromosome and within the Genome, Sujeet Kumar Mishra, Kunhe Li, Simon Brauburger, **Arnab Bhattacharjee**, Nestor Norio Oiwa, and Dieter Heermann, *Life*, 12, 541, 2022.
7. Kinetic Origin of Nucleosome Invasion by Pioneer Transcription Factors, Anupam Mondal, Sujeet Mishra and **Arnab Bhattacharjee***, *Biophysical Journal*, **120**, 5219-5230, 2021.
8. Mechanism of Dynamic Binding of Replication Protein A to ssDNA, Anupam Mondal and **Arnab Bhattacharjee***, *Journal of Chemical Information and Modelling*. **60**, 5057-5069, 2020.
9. 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 Bhattacharjee*** and Gobardhan Das, *Nature Cell Death and Disease*. **11**, 516, 2020.

10. 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 Bhattacharjee**, Manoj Munde, and Shailja Singh. *Biochemical Journal*, 477(12):2153-2177, 2020.

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

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

13. 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 Bhattacharjee***, *Soft Matter*. 15, 1960, 2019. The research is highlighted as Cover Page image of the journal.

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

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

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

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

18. Thermodynamic Protein Destabilization by GFP Tagging: A Case of Interdomain Allostery. Miri Sokolovski, **Arnab Bhattacharjee**, Naama Kessler, Yaakov Levy, Amnon Horovitz. *Biophysical Journal*, 109(6), 1157-1162, 2015.
19. Search by proteins for their DNA target site: 2. The effect of DNA conformation on the dynamics of multidomain proteins. **Arnab Bhattacharjee** and Yaakov Levy. *Nucleic Acid Research*, 42(20), 12415, 2014.
20. Search by proteins for their DNA target site: 1. The effect of DNA conformation on protein sliding. **Arnab Bhattacharjee** and Yaakov Levy. *Nucleic Acid Research*, 42(20), 12404, 2014.
21. Conformational properties and aggregation of the 1-93 fragment of apolipoprotein A-I. Jitka Petřlova, **Arnab Bhattacharjee**, Wouter Boomsma, Stefan Wallin, Jens Lagerstedt and Anders Irbäck. *Protein Science* 23(11), 1559, 2014.
22. Hybrid Monte Carlo with Non-Uniform Step Size. Christian Holzgräfe, **Arnab Bhattacharjee** and Anders Irbäck. *Journal of Chemical Physics*. 140, 044105, 2014.
23. Exploring protein-peptide binding specificity through computational peptide screening. **Arnab Bhattacharjee** and Stefan Wallin. *Plos Computational Biology* 9 (10), e1003277, 2013.
24. Coupled Folding-Binding in a Hydrophobic/Polar Protein Model: Impact of Synergistic Folding and Disordered Flanks. **Arnab Bhattacharjee** and Stefan Wallin. *Biophysical Journal*. 102, 569, 2012.
25. Role of Conformational Heterogeneity on Protein Misfolding. Anupaul Baruah, **Arnab Bhattacharjee** and Parbati Biswas. *Soft Matter* 8 (16), 4432, 2012.
26. Designing Misfolded Protein Sequences by Energy Landscaping. **Arnab Bhattacharjee** and Parbati Biswas. *Journal of Physical Chemistry B*. 115 (1), 113, 2011.
27. Role of Foldability and Stability in Designing Real Protein Sequences. **Arnab Bhattacharjee** 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).
28. Neutrality and Evolvability of Designed Protein Sequences. **Arnab Bhattacharjee** and Parbati Biswas. *Physical Review E*. 82, 011906, 2010. Also selected for 15th July 2010 issue of Virtual Journal of Biological Physics Research.

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

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

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

RESEARCH PUBLICATIONS UNDER REVISION/ACCEPTED

32. How Multiple Transcription Factors Recognize Their Binding Sites on Nucleosomal DNA ? Sujeet Kumar Mishra and **Arnab Bhattacharjee**, *ChemPhysChem*, 2022.

PRESENTATIONS/INVITED TALK AT MEETINGS

- *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.
- *Dancing on DNA: How proteins scan their target sites on DNA inside the cell* 1st Network Meeting, RTG Big Data Research, Allahabad University 2019.

- *How Protein Searches Target Sites on Nucleosomal DNA?* at 43rd Indian Biophysical Meeting , IISER Kolkata 2019.
- *Dancing on DNA* at Workshop on Bioinformatics and Molecular Modelling in Drug Design , BIF-MMDD, ACBR Delhi University 2019.
- *Looking into future through computers* at Human Resource Development Centre, UGC, Jawaharlal Nehru University 2019.
- *Dancing on DNA: How Proteins Scan their Target Sites on DNA?* Indian Association for Cultivation of Science 2018.
- *Role of Macromolecular crowding on the Intracellular diffusion of DNA Binding Proteins* at 42nd Annual Meeting of the Indian Biophysical Society (IBS 2018) at IISER Pune.
- Understanding the Role of DNA Topology in Target Search Dynamics of Proteins at 42nd Annual Meeting of the Indian Biophysical Society (IBS 2018) at IISER Pune.
- Role of DNA conformation in target search kinetics of DNA binding proteins. National Science Day at Jawaharlal Nehru University, 2018.
- *Can Computers Change Our Fate?* at Human Resource Development Centre, UGC, Jawaharlal Nehru University 2019.
- JAN-JAN-JNU Annual Open Day at Jawaharlal Nehru University 2017.
- *Searching Target Sites on DNA by Proteins: Role of DNA Dynamics under Confinement* at Annual Symposium of the Indian Biophysical Society (IBS 2017) at IISER Mohali.
- National Science Day 2017 at Jawaharlal Nehru University.
- *Exploring protein-peptide binding specificity through computational peptide screening* at NanoBio Interface, 2016 at Jawaharlal Nehru University.
- *Searching Target Sites on DNA by Proteins* at Instructional workshop on Computational Methods in Drug Discovery at Special Center for Molecular Medicine, Jawaharlal Nehru University.
- *Exploring protein-peptide binding specificity through computational peptide screening* International Conference on Biomolecular Simulations and Dynamics Recent Advances and Future Perspectives, IIT Madras, November 2013.
- *Intrinsically Disordered Proteins At Work: A simple Model Study.* Symposium on Dynamics of Bio-molecular Processes: From Atomistic Representations to Coarse-Grained Models. Stockholm, Sweden, 2012.

- *How Foldability and Stability Determines Mutational Robustness*, Symposium on Recent Trends in Biophysics, organized jointly by Tata Institute of Fundamental Research and Beneras Hindu University, at Varanasi 2010.
- *Statistical Theory of Neutral Protein Evolution by Random Site Mutations*, Theoretical Chemistry Symposium, IISc, Bangalore, 2009.
- *Statistical Theory of Protein Design Dynamics* Day Symposium organised by DU(Physics department) and JNU, 2009.
- *Statistical Theory of Combinatorial Protein Design by Energy Landscaping*, 10th CRSI Symposium, IISc, Bangalore, 2008.
- *Dynamics of Starburst Dendrimers with Stiff Spacers*, 9th CRSI Symposium, Delhi University, Delhi 2007.

RESEARCH PROJECTS UNDERTAKEN/ONGOING

- DST SERB Project titled *Invading Nucleosome: Understanding How Cells Recruit Proteins at Target DNA Sites* (CRG/2019/001001). - Ongoing (~ 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 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)

REVIEWER ASSIGNMENT

- Journal of Physical Chemistry B
- Biophysical Journal
- PLOS One
- Protein Science
- Soft Matter

- Polymers
- BMJ Open
- BMC Medical Genomics
- Scientific Reports
- Journal of Biomolecular Structure and Dynamics.

SUPERVISION

PHD

- Anupam Mondal
Thesis Title: *Understanding the Role of Structural and Functional Dynamics of DNA in Protein-DNA Recognition Using Theoretical and Computational Approaches.*
Present: **PostDoctoral position at Rice University, USA** with **Prof. Anatoly Kolomeisky.**
- Pinki Dey
Thesis Title: *Understanding the Role of Macromolecular Crowding on Target Search Dynamics of DNA Binding Proteins.*
Present: **Postdoctoral Fellow** with **Prof. John Mattick** in the School of Biotechnology and Biomolecular Sciences, University of New South Wales, Sydney, Australia.

PHD(ONGOING)

- Sujeet Kumar Mishra (M.Sc CompBio, SCIS).
Sujeet is also selected for a dual PhD program with Heidelberg university, Germany.
- Sangeeta Yadav (M.Sc in Chemistry, DU)
Sangeeta has been awarded the prestigious **Prime Minister's Research Fellowship (PMRF) in 2020** from **JNU.**
- Supervising Rahul Mittal (M.Sc Physics, IIT Mandi)
- Supervising Kavana Priyadarshi K (M.Sc in CompBio, SCIS).
- Supervising Anuradha Rajput (M.Sc Physics, JNU).
- Supervising Shrawan Chaudhury (M.Sc Biotechnology, IIT Bombay).

POSTDOCTORAL FELLOWS

- Pravin Kumar, Assistant Professor, Akal University, Punjab.
(2018-2019)

- Venkatramana Imandi,
(2019)

OTHERS

- Supervised Sakshi Khaiwal as project student at School of Computational and Integrative Sciences, Jawaharlal Nehru University. Currently a graduate student at University of Côte d'Azur, France.
- Supervised Prasant Chidella for B.Tech dissertation at IIT Delhi, India. Currently employed in Xerox, India.

TEACHING

- Teaching ***Statistical Mechanics of Complex Systems*** at School of Computational and Integrative Sciences, Jawaharlal Nehru University. (20 hours).
- Teaching ***Statistical Mechanics of Biomolecules and Simulations*** at School of Computational and Integrative Sciences, Jawaharlal Nehru University. (40 hours).
- Teaching ***Computational and Structural Biology*** at School of Computational and Integrative Sciences, Jawaharlal Nehru University (20 hours).
- Teaching ***Thermodynamics and kinetics*** at School of Computational and Integrative Sciences, Jawaharlal Nehru University. (13 hours).
- Teaching ***Numerical Techniques and simulation laboratory*** at School of Computational and Integrative Sciences, Jawaharlal Nehru University. (40 hours).
- Teaching ***Fundamentals of Data Structure and Computer Programming*** at School of Computational and Integrative Sciences, Jawaharlal Nehru University. (40 hours).
- Teaching ***Advanced topics in Physical Sciences*** at School of Computational and Integrative Sciences, Jawaharlal Nehru University. (40 hours).
- Taught ***Molecular Mechanics and Biological Physics*** at IIT Delhi, India. (40 hours).
- Taught ***Biophysics*** at IIT Delhi, India. (40 hours).

SYNERGISTIC ACTIVITIES

- 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.