Arnab Bhattacherjee

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PROFESSIONAL PROFILE

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

WORK HISTORY

Associate Professor, December 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

Broad Area: Understanding the structure-function relationship of **complex biological systems** that have long-term implications for combating medical conditions such as Creuzfeld-Jacob (Mad Cow disease), Alzheimer, and cancer by using **computational biology** techniques and **theoretical biophysical chemistry principles**. Current research interests include:

- Investigating the Nucleosome biophysics.
- The diffusion of molecular motors on biological track.
- Studying the growth kinetics and mechanism of nanocrystal formation.
- Probing transcription factor kinetics under various cellular condition.
- Role of molecular crowding on biomolecular interactions.
- Dynamics of disease-linked Intrinsically Disordered Proteins (IDPs) and their aggregation mechanisms.
- Investigating the protein-peptide interaction network.
- Sampling algorithms and effective force fields.
- Developing mesoscale models of various biopolymers in order to understand their folding/dynamics at molecular levels.

AWARDS/HONOURS/FELLOWSHIPS/GRANTS

- Joined Editorial Board of Biophysics as Review Editor for Frontiers in Physics, Frontiers in Physiology and Frontiers in Molecular Biosciences.

- Elected Associate of the Indian Academy of Sciences (IASc), August 2020 - December 2023.
- 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. 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.

2.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.

3.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.

4.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

5.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

6.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.

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

8. 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.

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

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

11.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.

12.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.

13.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.

14.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*.

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

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

17.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.

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

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

20.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).

21.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.

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

23.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.

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

PRESENTATIONS/INVITED TALK AT MEETINGS

- *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 RecentTrends 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)
- 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

- Supervising Anupam Mondal for PhD at School of Computational and Integrative Sciences, Jawaharlal Nehru University. Anupam has been awarded the prestigious **Ratna Phadke Award** from **Indian Biophysical Society** in 2018.

- Supervising Sujeet Kumar Mishra for PhD at School of Computational and Integrative Sciences, Jawaharlal Nehru University. Sujeet is also selected for a dual PhD program with Heidelberg university, Germany.

- Supervising Sangeeta for PhD at School of Computational and Integrative Sciences, Jawaharlal Nehru University. Sangeeta has been awarded the prestigious **Prime Minister's Research Fellowship (PMRF) in 2020** from **JNU**.

- Supervised Pinki Dey for PhD at School of Computational and Integrative Sciences, Jawaharlal Nehru University. Currently a **Postdoctoral Fellow** with **Prof. John Mattick** in the School of Biotechnology and Biomolecular Sciences, University of New South Wales, Sydney, Australia.

- 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 IIIT 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 Biomoleculs 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 IIIT Delhi, India. (40 hours).

- Taught ***Biophysics*** at IIIT 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, 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.