

# Sangeeta

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## Education

- July 2019 **Jawaharlal Nehru University, New Delhi**, Present *School of Computational & Intergrative Sciences*, Research Scholar (Computational Biology), Prime Minister's Research Fellow (PMRF). Supervisor: Dr. Arnab Bhattacherjee
- 2016 2018 University of Delhi, New Delhi, Department of Chemistry, Master in Science, Physical Chemistry Specialization.
- 2013 2016 **University of Delhi, New Delhi**, *Kalindi College*, Bachelor in Science, Chemistry Honours.

# **Research Interest**

Understanding the structure-function relationship of protein and Nucleic acid molecules using computational molecular biophysics techniques and mathematical models.

# Research Experience

## July 2019 - Jawaharlal Nehru University, Ph.D. Student.

- Ongoing My research is centred around the interaction between protein and Deoxyribonucleic acid (DNA) molecules, addressing the biophysical aspect of how single stranded DNA binding proteins transport on ssDNA trails. This research aims to understand the role of single stranded DNA binding proteins, in association with ssDNA, in the different genetic processes, for example, DNA replication, recombination and repair.
- July 2018 Jawaharlal Nehru University, Project Assistant.
- June 2019 Worked under the supervision of Dr. Arnab Bhattacherjee in the project entitled "Understanding the role of DNA flexibility in Protein-DNA recognitions".
- July 2017 University of Delhi, New Delhi, Masters Dissertation.
- May 2018 Masters Dissertation on *"Polymeric Nanoparticles in Cancer Therapy"* under the guidance of Prof. Indrajit Roy, Department of Chemistry, University of Delhi.

## September University of Delhi, New Delhi, Project Assistant.

2015 - May
2016 Project Assistant in the innovation project KC-302 Microbial Fuel Cell: An efficient benign set up for Electrochem 2016 ical Cell for removing of impurities from laboratory generated waste water under the guidance of Dr. Tarkeshwar (Department of Zoology, Kalindi College, University of Delhi) and Dr. Amit Kumar (Department of Chemistry, Jamia Millia Islamia University).

# Publications

- **2024 Sangeeta** and Arnab Bhattacherjee\*, "Exploring the protein-ssDNA binding specificity through computational ssDNA screening using Multisequence Hybrid Monte Carlo approach", manuscript under preparation, **2024**.
  - Babita Bisht, **Sangeeta**, Pinki Dey, Praveen Kujur, Avinash Singh, Shahnoor Ali, Sandeep, Sanjay Pant, Rana P. Singh, Mohan S. Mahata, "Insight into mechanism of non-radiative energy transfer via DY8-BSA complex: In vitro cytotoxicity studies" manuscript ready to communicate, **2024**.
  - **Sangeeta** and Arnab Bhattacherjee<sup>\*</sup>, "The Importance of Nick in Protein Target Search Dynamics on Supercoiled DNA", Communicated, **2024**.

- **Sangeeta**, Sujeet Kumar Mishra and Arnab Bhattacherjee\*, "Role of shape deformation of DNA binding sites in regulating the efficiency and specificity in their recognition by DNA binding proteins ", accepted in JACS Au, **2024** (doi: 10.1021/jacsau.4c00393).
- Shrawan Kumar Choudhary<sup>‡</sup>, Sangeeta<sup>‡</sup> Pinki Dey, and Arnab Bhattacherjee<sup>\*</sup>, "Modeling Facilitated Diffusion of Proteins in Crowded Environment", accepted, Springer, 2024 (<sup>‡</sup>These authors contributed equally) (Book Chapter).
- Sujeet Kumar Mishra, **Sangeeta**, Dieter W. Heermann and Arnab Bhattacherjee\*, "The Role of Nucleotide Opening Dynamics in Facilitated Target Search by DNA-Repair Proteins", **BBA Gene Regulatory Mechanisms**, 1867(2), 195026, **2024**.
- Harsh Bhardwaj, Vani Jhalani, Anupam, Sangeeta\*, "COVID-19, pandemics and epidemics in general:An epidemiological and historical account", accepted in *International Conference on Next Generation Digital Technologies*, 2024 (\*Corresponding Author).
- Sumiran Kumar Gurung, **Sangeeta**, Priyanka Dubey, Abhik Saha, Fatima Akhtar, Arnab Bhattacherjee\* and Suman Kumar Dhar\*, "Unusual weak and delayed GTPase activity of FtsZ from human pathogenic bacteria *Helicobacter pylori*", **The Journal of Biochemistry**, 75(4):405–417, **2024**.
- 2023 Sangeeta, Arnab Bhattacherjee\*, "Unraveling the molecular basis of protein search on ssDNA track and binding specificity of the ssDNA sequences", Biophysical Journal, 122(3), SUPPLEMENT 1, 215a, Conference Abstract, 2023.
  - **Sangeeta** and Arnab Bhattacherjee\*, "Interdomain dynamics in human Replication Protein A regulates kinetics and thermodynamics of its binding to ssDNA", **PLoS ONE**, 18(1):e0278396, **2023**.
  - **Sangeeta**, Shilpi Khurana, Amit Kumar, "Translational transport of e-waste and implications on human well beings and the environment", Elsevier, **2022**, 125-142 (Book Chapter).
- **2022** Anupam Mondal, **Sangeeta**, Arnab Bhattacherjee\*, "Torsional behaviour of supercoiled DNA regulates protein–DNA recognition", **Nucleic Acids Research**, 50(12):6671–6686, **2022**.
- **2021 Sangeeta**, Poorna Khanna, Kapinder, Tarkeshwar, Amit Kumar, "Microbial fuel cell: a greener way to protect the environment", Academic Press, **2021**, 575-584 (Book Chapter).
  - Pinki Dey, **Sangeeta**, "Review of: "Impact of crowded environments on binding between protein and single-stranded DNA", Qeios, CC-BY 4.0, **2021**, https://doi.org/10.32388/9D6S2W (Qeios Review).

## Relevant Courses

Ph.D. Research Methodology, Biomolecular Simulation, Numerical Techniques and Programming, Reading Courses Course (Literature Survey), Python

#### Skills

- Communication, Leadership, Teamwork
- Strong reading, writing and speaking competencies for English and Hindi
- C language, Python, Molecular Dynamics, Monte Carlo
- Gromacs, Pymol, Visual Molecular Dynamics (VMD), Chimera
- MS Office, Latex (overleaf), WIX website design, iOS, Windows, Linux

# Awards/Honours/Fellowships

- **Received International Travel Grant** under SERB International Travel Scheme for attending 21<sup>st</sup> IUPAB Congress 2024 at Kyoto, Japan in June, 2024 (**May, 2024**).
- CHPHI Elsevier Award for best poster presentation at Physical Chemistry Symposium 2023 (SoPhyC-2023) organized by Society of Physical Chemistry (SoPhyC) and Department of Chemistry, IIT Kanpur (October, 2023)
- Best Oral Presentation Award at 4th Annual Ph.D. Symposium held at School of Computational & Integrative Sciences, Jawaharlal Nehru University, New Delhi (October, 2023)
- Receiving Prime Minister Research Fellowship, Ministry of Human Resource Development (MHRD), Government of India (2020 Onward)

- Recipient of Prime Minister Research Fellowship, Ministry of Human Resource Development (MHRD), Government of India (2020)
- Received Junior Research Fellowship, Council of Scientific & Industrial Research (CSIR) (2019-2020)
- Ranked 58 in JRF in Chemical Science, Council of Scientific & Industrial Research (CSIR) (June, 2018)
- Received offer letter for DST Inspire fellowship under Assured Opportunity for Research Careers (2018)
- Scored 1<sup>st</sup> Rank in Bachelors in Chemistry, Kalindi College, University of Delhi (2013-2016)
- First Prize in Poster Presentation at National Symposium on *"Trends in Research and Innovations in Life Sciences at Undergraduate Level"* held at Deen Dayal Upadhyaya College, University of Delhi (2016)
- DST Inspire Scholarship for acquiring good academic marks in 12th standard in Haryana Board (2013 - 2018)

## Conferences and Workshops

- 2023 Poster Presentation at Physical Chemistry Symposium 2023 (SoPhyC-2023) organized by Society of Physical Chemistry (SoPhyC) and Department of Chemistry, IIT Kanpur (October, 2023)
  - **Oral Presentation** at 4th Annual Ph.D. Symposium held at School of Computational & Integrative Sciences, Jawaharlal Nehru University, New Delhi (**October, 2023**)
  - PMRF Review Presentation entitled "Molecular Trafficking on DNA: How Computers Can Help to Break Transcription Code" under Prime Minister Research Fellowship (PMRF) Review 2023 (June, 2023).
  - **Poster Presentation** at Biophysical Society (BPS) Annual Meeting 2023 held at San Diego Convention Center, San Diego, United State of America (**February, 2023**)
- 2022 Student Talk at *Molecular Simulation: Focus on Method* held at Tata Institute of Fundamental Research, Hyderabad, India (December, 2022)
  - Short Talk at Statistical Biological Physics: From Single Molecule to Cell Program held at International Centre for Theoretical Sciences, Tata Institute of Fundamental Research, Bengaluru, India (October, 2022).
  - **Flash Talk and Poster Presentation** at India | EMBO Lecture Course *Functional nucleic acids: Recent landscapes and therapeutic applications* held at Regional Centre of Biotechnology, Faridabad, India in the hybrid mode (**August, 2022**).
  - PMRF Review Presentation entitled "Molecular Trafficking on DNA: How Computers Can Help to Break Transcription Code" under Prime Minister Research Fellowship (PMRF) Review 2022 (May, 2022).
  - **E-Poster Presentation** at the Conference IBS-2022 *Conceptual Advances in Biophysics and its Applications* held at ACTREC, Tata Memorial Centre, Navi Mumbai in the hybrid mode (**March, 2022**).
- 2021 PMRF Review Presentation entitled "Shielding ssDNA and maintain Genomic Integrity: How do cells achieve that??" under Prime Minister Research Fellowship (PMRF) Review 2021 (December, 2021).
  - Participated in the Conference SMCB 2021 Statistical Mechanics in Chemistry and Biology (2021).
  - Participated in the International Conference on MSMM'21 (ONLINE) Multiscale Simulation & Mathematical Modelling of Complex Biological Systems organized by Jawaharlal Nehru University, New Delhi (March, 2021).
- 2020 Participated in International Conference, ICTS program, on *Statistical Biological Physics: From Single Molecule to Cell (Online)* organized by Tata Institute of Fundamental Research, Bengaluru (December, 2020).
  - Participated in AAJ series webinar on *Self Reliant India: Aspirations & Opportunities* organized by Jawaharlal Nehru University (2020).

- Participated in The First Online India-UK Bilateral SPARC symposium on *Transcriptional Dynamics* in *Developmental Biology* organized by SciWhyLab, School of Computational & Integrative Sciences (SC&IS), Jawaharlal Nehru University (JNU), New Delhi, India, (2020).
- Participated in a workshop on *DNA Bubble Formation: From Physics to Biological Functions* held at Department of Physics, Banaras Hindu University, Varanasi (**February, 2020**).
- 2019 Paper Presentation at National Conference on *Recent Advances in Agriculture, Food Tech and Human Health* held at Sam Higginbottom University of Agriculture, Technology and Sciences, Prayagraj (November, 2019).
  - Participated in Pre-Conference workshop on *Multiscale Simulation & Mathematical Modelling of Complex Biological Systems* held at Jawaharlal Nehru University, New Delhi (**January, 2019**).
  - **Poster Presentation** at International Conference cum workshop on *Multiscale Simulation & Mathematical Modelling of Complex Biological Systems* held at Jawaharlal Nehru University, New Delhi (January, 2019).
- 2018 Participated in a workshop on *InCOB 2018 Workshop On Programmatic Access to Protein Sequence, Function and Structure with UniProt and PDBe* held at Jawaharlal Nehru University, New Delhi (2018).
  - Participated in International Conference on *Emerging Trends in Drugs Development and Natural Products (ETDDNP-2018)* held at Department of Chemistry, University of Delhi, New Delhi (**2018**).
- **2017** Participated in workshop on *Skill Training Programme in Science Communication, Science Journalism and Scientific Writing* organized by University of Delhi, New Delhi and NISCAIR, New Delhi (**2017**).
  - Participated in Indo-EU Workshop on *Electrochemical Technologies* held at Department of Chemical Engineering, IIT Delhi, New Delhi (**2017**).
  - **Poster Presentation** at National Seminar on *A Paradigm Shift Towards Empowerment of Women* held at Kalindi College, University of Delhi, New Delhi (**2017**).
- 2016 Participated in National Symposium on *Environment: Greener Future & Awareness* held at Deshbandhu College, University of Delhi, New Delhi (2016).
- 2015 Paper Presentation at Inter College Fest SCINTILLATIONS 2015 held at Gargi College, University of Delhi, New Delhi (2015).

## Extra Curricular Activites

- March, 2024 **Student Coordinator, Jawaharlal Nehru University**. Student Coordinator of One-day Symposium titled *Simulations of Physical and Biological Systems* held at Jawaharlal Nehru University, New Delhi.
- April, 2023 Teaching Assistant, Department of Chemistry, Jamia Millia Islamia, New Delhi.

Dec, 2023 Taught *Chemistry* at the Department of Chemistry, Jamia Millia Islamia (A Central University), New Delhi.

October, Convener, Jawaharlal Nehru University.

2023 Convener of 4th Annual Ph.D. Symposium held at School of Computational & Integrative Sciences, Jawaharlal Nehru University, New Delhi.

- September, Participation in IFP Season 12.
  - 2022 Participated in World's Largest Filmmaking Challenge IFP 50 Hour Filmmaking Challenge at IFP Season 12.
- April, 2022 Teaching Assistant, Ramjas College, University of Delhi.
- March, 2023 Taught *Physical Chemistry* to undergraduate students at Ramjas College.
- May, 2022 Volunteer, Jawaharlal Nehru University.

Participated as volunteer in *Scientegration 2022* held at School of Computational & Integrative Sciences, Jawaharlal Nehru University, New Delhi (**2022**).

- Sept, 2021 Teaching Assistant, Hansraj College, University of Delhi.
- March, 2022 Taught Research Writing and Communication Skill Management course to undergraduate students at Hansraj College.

#### March, 2021 Student Coordinator, Jawaharlal Nehru University. Student Coordinator of International Conference on *Multiscale Simulation and Mathematical Modelling of Complex Biological Systems (MSMM'21)* held at Jawaharlal Nehru University, New Delhi in online mode.

#### January, 2019 Student Coordinator, Jawaharlal Nehru University.

Student Coordinator of International Conference cum Workshop on *Multiscale Simulation and Mathematical Modelling of Complex Biological Systems (MSMM'19)* held at Jawaharlal Nehru University, New Delhi.

#### 2015 - 2016 **Society President, Biochemical Society, Kalindi College**. Worked as President at Biochemical Society, Kalindi College, University of Delhi, New Delhi.

#### 2015 **Volunteer, Kalindi College, University of Delhi**. Participated as Volunteer in Annual Inter College Fest *LEHREN-2015* held at Kalindi College, University of Delhi, New Delhi.