

Born on October 1993 in India. Known languages are English, Hindi, and Bengali. Citizenship Indian.

## CURRENT POSITION

- Postdoctoral fellow at the Max Planck Institute for Polymer Research since 1st February 2023. Advisor: Dr. Oleksandra Kukharenko and Prof. Kurt Kremer.

## WORK EXPERIENCE

- Postdoctoral fellow at the ICGM, University of Montpellier, CNRS, ENSCM, Montpellier, France from 1st January 2022 to 31st January 2023. Advisor: Prof. Guillaume Maurin.
- Research Associate at the Center for Condensed Matter Theory, Department of Physics of the Indian Institute of Science from August 2021 to December 2021. Advisor: Prof. Prabal K. Maiti.

## EDUCATION

- **Ph.D.** Aug 2016 — Nov 2021  
Center for Condensed Matter Theory  
Department of Physics, Indian Institute of Science Bangalore India  
Ph.D. Thesis Title: Multiscale Modelling of Nucleic Acid Nanostructures.  
Advisor: Prof. Prabal K. Maiti.
- **M.S.(Physics),** 2014—2016  
Department of Physics, Indian Institute of Technology Bombay, India  
M.S. Thesis Title: A Tug-of-War model for transport of cargo by molecular motors and catch bond mechanism in dynein motors.  
Advisor: Prof. Mithun K. Mitra.
- **B.Sc., Physics (Major), Mathematics, Chemistry,** 2011—2014  
Department of Physics,  
Presidency University, Kolkata, India.

## AREAS OF RESEARCH

- Statistical Physics
- Computational Physics
- Polymer Physics
- Soft Condensed Matter
- Biological Physics
- Material Science

## BRIEF SUMMARY OF RESEARCH

I strive to understand the physical principles that govern the microscopic world around and within me. My research is primarily focused on the quantification of the statistical properties of nano-materials and elucidating the underlying physics behind the spatial and temporal organization of biomolecules in cells. To achieve this, I employ an integrative approach combining multiscale molecular simulations, data-driven machine learning techniques and theory from equilibrium and non-equilibrium statistical mechanics. Currently, I am trying to understand how ubiquitin and SUMO affect the propensity of target proteins containing intrinsically disordered regions to undergo phase separations and aggregation. In my previous postdoctoral work, I employed a multiscale methodology that involved Density-functional theory, Molecular dynamics, and Grand-canonical Monte Carlo to model polymer melts and metal-organic frameworks to explore their perm-selectivity properties. During my Ph.D., I investigate the structure, dynamics, and thermodynamics of nucleic acids from the viewpoint of classical statistical physics. Alongside my current research work, I am interested in analytical approaches to equilibrium and non-equilibrium phenomena in complex systems.

## PUBLICATIONS (9 FIRST-AUTHORED AND 8 CO-AUTHORED)

1. **Supriyo Naskar**, Himanshu Joshi, Banani Chakraborty, Nadrian C Seeman, Prabal K Maiti. "Atomic Structures of RNA nanotubes and comparison with DNA nanotubes", *Nanoscale*, 2019, 11 (31), 14863-14878.
2. Palka Puri, Nisha Gupta, Sameep Chandel **Supriyo Naskar**, Anil Nair, Abhishek Chaudhuri, Mithun K Mitra, Sudipto Muhuri. "Dynein catch bond as a mediator of codependent bidirectional cellular transport", *Physical Review Research* 2019, 1 (2), 023019.
3. **Supriyo Naskar**, Mounika Gosika, Himanshu Joshi, Prabal K Maiti. "Tuning the Stability of DNA Nanotubes with Salt", *Journal of Physical Chemistry C*, 2019, 123 (14), 9461-9470.
4. **Supriyo Naskar**, Suman Saurabh, Yun Hee Jang, Yves Lansac, Prabal K Maiti. "Liquid crystal ordering of nucleic acids" *Soft Matter*, 2020, 16 (3), 634-641

5. Abhishek Aggarwal\*, **Supriyo Naskar**\*, Anil Kumar Sahoo\*, Santosh Mogurampelly, Ashok Garai, Prabal K Maiti. “What do we know about DNA mechanics so far?” *Current Opinion in Structural Biology* 2020, 64, 42-50. \*Equal Contribution.
6. **Supriyo Naskar**, Prabal K Maiti. “Mechanical properties of DNA and DNA nanostructures: comparison of atomistic, martini and oxDNA”, *Journal of Materials Chemistry B*, 2021, 9 (25), 5102-5113.
7. Abhishek Aggarwal\*, **Supriyo Naskar**\*, Nikhil Maroli\*, Biswajit Gorai, Narendra M Dixit, Prabal K Maiti. “Mechanistic Insights into the Effects of Key Mutations on SARS-CoV-2 RBD-ACE2 Binding”, *Physical Chemistry Chemical Physics*, 2021, 9 (25), 5102-5113.\*Equal Contribution.
8. Vinod Morya, Shanka Walia, Ankit Gangrade, **Supriyo Naskar**, Aditya Guduru Teja, Sameer Dalvi, Prabal K Maiti, Chinmay Ghoroi, Dhiraj Bhatia. “Designer DNA hydrogels to stimulate 3d cell invasion by enhanced receptor expression and membrane endocytosis”, *ACS Biomaterials Science & Engineering*, 2021, 7(12), 5933-5942.
9. Khadka B Chetri, Akshar Sharma, **Supriyo Naskar**, Prabal K Maiti, “Nanoscale structure and mechanics of peptide nucleic acids”, *Nanoscale*, 2022,14, 6620-6635.
10. **Supriyo Naskar**, Anil Kumar Sahoo, Mohd Moid, Prabal K Maiti. “Ultra-high permeable phenine nanotube membranes for water desalination”, *Physical Chemistry Chemical Physics*, 2022, 24, 11196-11205.
11. Subrata Pandit, Nikhil Maroli, **Supriyo Naskar**, Bhavesh Khatri, Prabal K Maiti, Mrinmoy De, “Graphene Oxide as a Dual Template for Induced Helicity of Peptides”, *Nanoscale*, 2022, 14, 7881-7890.
12. Khadka B Chetri, **Supriyo Naskar**, Prabal K Maiti. “Probing the microscopic structure and flexibility of oxidized DNA by molecular simulations”, *Indian Journal of Physics*, 2022, 96, 2597-2611.
13. Abhishek Aggarwal, **Supriyo Naskar**, Prabal K Maiti, “Molecular rectifiers with very high rectification ratio enabled by oxidative damage in double-stranded DNA”, *Journal of Physical Chemistry B* 2022, 126, 4636-4646.
14. **Supriyo Naskar**, Dhiraj Bhatia, Shiang-Tai Lin, Prabal K Maiti. “Mechanistic insight into the structure, thermodynamics and dynamics of equilibrium gels of multi-armed DNA nanostars”, *Physical Chemistry Chemical Physics*, 2023, 25, 7847-7858.
15. **Supriyo Naskar**, Dong Fan, Aziz Ghoufi, Guillaume Maurin, “Microscopic insight into the shaping of MOFs and its impact on CO<sub>2</sub> capture performance”, *Chemical Science*, 2023, 14, 10435-10445.
16. Karuppasamy Gopalsamy, Dong Fan, **Supriyo Naskar**, Yann Magnin, and Guillaume Maurin, “Engineering of an Isoreticular Series of CALF-20 Metal–Organic Frameworks for CO<sub>2</sub> Capture”, *ACS Applied Engineering Materials*, 2024.
17. Dong Fan, **Supriyo Naskar**, and Guillaume Maurin, “Unconventional mechanical and thermal behaviors of MOF CALF-20”, *Arxiv Preprint 2024*, In review at *Nature Communications*.

## MANUSCRIPT UNDER PROCESS

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- R. Hardian, J. Jia, A. Diaz, **Supriyo Naskar**, D. Fan, O. Shekhah, G. Maurin, M. Eddaoudi, G. Szekely, “Design of mixed-matrix membranes with asymmetric filler density and intrinsic compatibility for improved molecular sieving”, To be submitted.
- **Supriyo Naskar**, Dong Fan, Guillaume Maurin, “Ultra-high perm-selective polymers for gas separation”, To be submitted.

## OTHER PUBLICATION

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- **Supriyo Naskar** “Multiscale Simulation of Nucleic Acid Nanostructures”, *Indian Institute of Science*, 2021.

## TALKS AND POSTER PRESENTATIONS

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- “Poster Day”, Max Planck Institute of Polymer Research, 2023.
- “SFB 1551 retreat”, Germany, October 2023.
- “Scientific advisory board meeting”, Max Planck Institute of Polymer Research, 2023.
- “Open Oral Presentation”, Indian Institute of Science, Bangalore, India, November, 2021.
- “Thesis Colloquium”, Indian Institute of Science, Bangalore, India, July, 2021.
- “Mainz Materials Simulation Days, Poster Presentation”, June, 2021.
- “RSC-IISER Desktop Seminar Poster Presentation”, May, 2021.
- “ACS Spring Meeting”, Virtual Meeting, April, 2021.
- “RSC Twitter Poster Presentation”, March, 2021.
- “RSC Materials Chemistry Division poster symposium”, Virtual Meeting, January, 2021.
- “Dr. K V Rao Research Awards Talk”, Hyderabad, India, August, 2020.
- “Informal Virtual APS meeting for self-limiting assemblies”, USA, March, 2020.
- “6 th Indian Statistical Physics Community Meeting” at International Centre for Theoretical Sciences, Tata Institute of Fundamental Research, Bangalore, India, February 2019.
- “Dynamics at the Interface of Chemistry and Biology” at Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore, India, February 2019.
- “Inhouse Symposium” at Department of Physics, Indian Institute of Science, Bangalore, India, November 2019.
- “Inhouse Symposium” at Department of Physics, Indian Institute of Science, Bangalore, India, November 2018.
- “Inhouse Symposium” at Department of Physics, Indian Institute of Science, Bangalore, India, November 2017.

## AWARDS & HONORS

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- International Travel award to attend APS March Meeting by Department of Science and Technology, 2020.
- Senior Research Fellowship Awarded by Council of Scientific & Industrial Research (CSIR), India in August 2018-July 2021.
- Junior Research Fellowship Awarded by CSIR, India in August 2016-July 2018.
- Qualified Graduate Aptitude Test in Engineering, 2016.
- Qualified Joint Entrance Screening Test, 2016.
- Qualified CSIR National Eligibility TEST, December 2015.
- Qualified CSIR Lectureship, June 2015.
- Awarded Innovation in Science Pursuit for Inspired Research (INSPIRE) Scholarship 2011-2016 by the Department of Science and Technology India.

## TEACHING EXPERIENCE

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- Teaching assistant for the course “Quantum Mechanics PH203” taught by Prof. Diptiman Sen during August to December 2018 at Indian Institute of Science, Bangalore, India.
- Taught the “Delay Differential equation” topic for the course “Advanced Simulation Technique” taken by Prof. Punit Parmananda in 2016.

## MENTORING

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- Akshar Sharma, MS Project at IISc, 2018-2019 under the guidance of Principal Investigator Prof. Prabal K Maiti.
- Khadka B Chetri, PhD at IISc, 2019-2021 under the guidance of Principal Investigator Prof. Prabal K Maiti.

## TECHNICAL SKILLS

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<b>Numerical Techniques:</b>	Statistical Mechanics, Molecular Dynamics and Monte Carlo Simulations, Free-Energy and Entropy Calculations, Density Functional Theory, Coarse-Grain modelling.
<b>Programming Languages:</b>	Python, Fortran, Tcl, Shell Scripting, C.
<b>Softwares:</b>	AMBER, NAMD, GROMACS, LAMMPS, Gaussian, Avadrado, oxDNA, caDNAno, MD Studio, HOOMD.
<b>Visualization Tools:</b>	VMD, Pymol, Chimera, Xmgrace, gnuplot, GIMP, Inkscape.
<b>High-Performance Computing:</b>	Maintaining Clusters, Installing Softwares, Running Jobs.

## PEER REVIEW

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- Langmuir, ACS Omega, Journal of Biomolecular Structure and Dynamics.

## REFERENCES

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- **Prof. Kurt Kremer**  
Polymer Theory,  
Max Planck Institute for Polymer Research,  
Ackermannweg 10, 55128 Mainz, Germany  
E-mail: kremer@mpip-mainz.mpg.de  
Website, Google Scholar
- **Prof. Prabal K Maiti**  
Centre for Condensed Matter Theory  
Department of Physics  
Indian Institute of Science  
Bangalore 560012, India  
E-mail: maiti@iisc.ac.in  
Website, Google Scholar  
Phone: +91 80 2293 2865
- **Dr. Oleksandra Kukharenko**  
Polymer Theory,  
Max Planck Institute for Polymer Research,  
Ackermannweg 10, 55128 Mainz, Germany  
E-mail: kukharenko@mpip-mainz.mpg.de  
Website, ORCID.
- **Prof. Guillaume Maurin**  
Institute Charles Gerhardt,  
University of Montpellier,  
École Nationale Supérieure de Chimie Montpellier,  
Centre National de la Recherche Scientifique  
34090 Montpellier, France  
E-mail: guillaume.maurin1@umontpellier.fr  
Google Scholar.