

CONTACT INFORMATION	52 Scribner Avenue Staten Island New York, USA Tel: +1(347)698-6383	Homepage: Click Here Google Scholar: Click Here GitHub: abhik-compbio ✉ E-mail: ghoshabhik.physics@gmail.com
RESEARCH INTEREST	<ul style="list-style-type: none"> • Structural & dynamical properties of bio molecules like protein. • Conformational thermodynamics & enhanced sampling. • Dynamics of hydration water. • Application of machine learning in biomolecular simulations. • Allostery. • Protein-ligand interactions. • Coarse grained modelling of biomolecules. 	
WORK EXPERIENCE	Postdoctoral Research Associate in College of Staten Island, City University of New York, USA (May 2023– Present) <ul style="list-style-type: none"> • Advisor: Prof. Sharon Loverde. • Area of research: Development of computational methods to probe the structure and stability of the nucleosome core particle using all atom and coarse grained simulation. 	
EDUCATION	Ph.D. in Theoretical soft matter physics (March 2023):S.N.Bose National Centre For Basic Sciences , Kolkata, India. <ul style="list-style-type: none"> • Advisor: Prof. Jaydeb Chakrabarti. • Thesis title: Microscopic insights to the relaxation phenomena in proteins (Degree awarded: February 2024). • Coursework completed: Advanced equilibrium statistical mechanics, Numerical methods & Fundamentals of Biophysics. M.Sc. in Physics (2015-2017):Ramakrishna Mission Vivekananda Educational Research Institute , India. <ul style="list-style-type: none"> • Advisor: Dr. Shamik Gupta. • Project thesis title: <i>Two dimensional Ising model solution using Onsager's Matrix method</i> • CGPA: 9.11/10 • Relevant courses: Statistical mechanics, Quantum mechanics, Mathematical methods, Condensed matter physics, Computational Physics etc. B.Sc. (Honours) in Physics (2012-2015):University Of Burdwan , India. <ul style="list-style-type: none"> • Subjects: Major in Physics, with Chemistry and Mathematics as auxiliary subjects • Marks: 65 % in Physics (1st Class). 	
MANUSCRIPT ACCEPTED	<ol style="list-style-type: none"> 1. Sequence Dependence in Nucleosome Dynamics, Prabir Khatua , Abhik Ghosh Moulick, Phu K Tang, Rutika Patel , Anjela Manandhar, Sharon Loverde, <i>J. Phys. Chem. B</i> 2024, 128, 13, 30903101. 2. Fluctuation dominated ligand binding in molten globule protein, Abhik Ghosh Moulick & J. Chakrabarti, <i>J. Chem. Inf. Model.</i> 2023, 63, 17, 55835591. 3. Conformational fluctuations in molten globule state of α-lactalbumin, Abhik Ghosh Moulick & J. Chakrabarti, <i>Phys. Chem. Chem. Phys.</i>, 2022, 24, 21348. . 4. Correlated dipolar and dihedral fluctuation in a protein, Abhik Ghosh Moulick & J. Chakrabarti, <i>Chemical Physics Letters</i>, 13874 (2022) 5. Correlation between protein bond vector and dihedral fluctuations, Abhik Ghosh Moulick & J. Chakrabarti, <i>AIP Conference Proceedings</i> 2265, 030036 (2020) . 	

MANUSCRIPT IN PREPARATION	<ol style="list-style-type: none"> 1. A.G. Moulick, Anirban Paul, J. Chakrabarti, Coarse-grained model of protein with structural information. 2. A.G. Moulick Dynamics of water at protein-ligand interface in molten globule state. 3. A.G. Moulick, P Khatua, R Patel, A Onyema, S M Loverde, Comparative exploration of nucleosome dynamics, using all-atom and coarse-grained approaches. 	
COMPUTATIONAL SKILL & SOFTWARES	<ul style="list-style-type: none"> • <i>Operating System:</i> MacOS, Linux - Ubuntu. • <i>Programming Languages:</i> Fortran, Python, R(Basic). • <i>Softwares:</i> Gromacs, NAMD, Amber, LAMMPS, PLUMED. 	<ul style="list-style-type: none"> • <i>Visualisation and analysis :</i> VMD,Pymol • <i>HPC Experience:</i> CRAY (SNBNCBS), CUNY-HPC, PSC • <i>Others:</i> GNUPLOT, XMGrace, Latex, Lyx, Shellsript
SKILLS & TECHNIQUES	<ul style="list-style-type: none"> • Classical all atom Molecular Dynamics. • Analysis of time dependent cross correlation functions. • Numerical analysis e.g. Gaussian quadrature e.t.c. • Constant pH molecular dynamics in implicit & explicit solvent. • Clustering (Geometrical clustering, Density based cluystering). 	<ul style="list-style-type: none"> • Machine learning model (XGBoost). • Protein-ligand docking. • Enhanced sampling. • Self-Van Hove function, Mean Squared Displacement, Survival probability. • Monte carlo simulation. • Bead-spring polymer model.
TALK DELIV- ERED/ORAL PRESENTATION	<ol style="list-style-type: none"> 1. Microscopic Understanding of Fatty Acid Binding with α-Lactalbumin at Molten Globule State. In:Hunfeld 2023: Hybrid Workshop on Computer Simulation and Theory of Macromolecules, Organized by Max Planck Institute for Multidisciplinary Sciences, Germany, 28.04.2023-29.04.2023. 2. Coarse-grained model of protein with structural informations. In:Steady State Phenomena In Soft Matter, Active and Biological Systems, Organized by S N Bose National Centre for Basic Sciences, 16.03.2023-18.03.2023. 3. Molecular insights into the binding of fatty acids with α-Lactalbumin at the molten globule (MG) state. In: Bose Fest 2023, Organized by S N Bose National Centre for Basic Sciences. 4. Conformational fluctuations in molten globule (MG) state of α-lactalbumin. In: Data Modeling and Computation: Capturing Biomolecular Processes, organised by CECAM, Lausanne, Switzerland, 31.10.2022-04.11.2022. 5. Functionality of protein at Molten Globule (MG) state. In: School of Biotechnology, Jawaharlal Nehru University (JNU), New Delhi, Host: Dr. Jaydeep Bhattacharya, October, 2022. 6. Biology under computational microscope, in the occasion of national science day at SNBNCBS, February 2022. 	
CONFERENCE POSTERS	<ol style="list-style-type: none"> 1. Comparative exploration of DNA dynamics in Nucleosome Core Particle using all-atom and coarse-grained approaches. In: CECAM Workshop at ENS Lyon France, 2024. 2. Comparative exploration of DNA dynamics in Nucleosome Core Particle using all-atom and coarse-grained approaches. In: Biophysical Society Annual Meeting, Philadelphia, 2024. 3. Microscopic understanding of fatty acid binding with α-lactalbumin at molten globule state. In: MBU@50, Organized by Molecular Biophysics Unit, IISc Bangalore. 4. Conformational fluctuations in molten globule (MG) state of α-lactalbumin (aLA). In: ID-Posters22, Organized by IDPSeminars (Virtual). 5. Conformational fluctuations and binding in molten globule (MG) state of alpha-lactalbumin (aLA) protein. In: Bose Fest 2022, Organized by S N Bose National Centre for Basic Sciences. 	

6. Functional characterisation of molten globule state of protein based on microscopic simulations. In: Recent Advances in Modelling Rare Event (RARE-2021) organized by IIT Kanpur, December 2021 (Virtual).
7. Correlated dipolar and dihedral fluctuation in a protein. In : ChemSci2021 organized by JN-CASR and RSC, December 2021 (Virtual).
8. Correlated dipolar and dihedral fluctuation in a protein. In: Bose Fest 2020, Organized by S N Bose National Centre for Basic Sciences.
9. Correlation between protein bond vector & dihedral fluctuations. In : DAE Solid State Physics Symposium, IIT Jodhpur, December 2019.
10. Correlation between protein bond vector & dihedral fluctuations. In : StatPhys Kolkata - X, Presidency University, Kolkata, November 2019.

WORKSHOP/ SCHOOL ATTENDED

1. i-CoMSE Workshop: Machine Learning for Molecular Science, University of Minnesota, Twin Cities, July 2023.
2. Statistical Biological Physics: From Single Molecule to Cell, International Centre For Theoretical Sciences, December 2020 (Virtual).
3. Mini school on Computational Physical Sciences in ACTSM 2020, S. N. Bose National Centre For Basic Sciences, February 2020.
4. Workshop on Advanced Simulation Methods: DFT, MD & Beyond (ASM 2019), IIT Delhi, March 2019.
5. National Summer School on statistical physics, S. N. Bose National Centre For Basic Sciences, June 2018.

HONORS AND AWARDS

1. Received CUNY Postdoctoral Travel award to attend Biophysical Society Annual Meeting 2024 at Philadelphia, USA.
2. Received Department of Biotechnology (DBT), Government of India Travel Award for attending International conference organized by CECAM, 2022.
3. Received Council of Scientific & Industrial Research (CSIR), Government of India Travel Award for attending International conference organized by CECAM, 2022.
4. Selected for INSPIRE Fellowship for PhD funded by Department of Science & Technology, Government of India, April, 2018-April, 2023.
5. Qualified SET 2018, UGC Accredited state eligibility test for post of Assistant Professor in the West Bengal, India.
6. Qualified in Joint Entrance Screening Test (JEST) 2015 & 2018, a test conducted for selecting candidates to be interviewed for admission to PhD Programmes in Physics / Theoretical Computer Science in various reputed institutions in India.
7. Qualified in Graduate Aptitude Test in Engineering (GATE) 2017 & 2018, a national level competitive examination, conducted by the Indian Institute of Technology (IIT).
8. Qualified in Joint Admission Test for M.Sc (JAM) 2015, a national level competitive examination, conducted by the Indian Institute Of Technology (IIT).
9. Qualifies NGPE-2014 conducted by Indian Association Of Physics Teachers (Placed among National top 1% candidate.)
10. Awarded INSPIRE Scholarship By Ministry of Science and Technology, Government of India for ranking among the top 1% in 12th standard Board Examinations and pursuing courses in Natural and Basic sciences at the B.Sc. and M.Sc. levels (2012-2017).

PERSONAL INFORMATION

- Birth: August 18, 1993
- Nationality: Indian
- Marital Status: Married

REFERENCES Prof. Sharon Loverde
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DECLARATION I, Abhik Ghosh Moulick, hereby declare that all the information given above is true and correct to the best of my knowledge.

SIGNATURE *Abhik Ghosh Moulick.*