CURRICULUM VITAE

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ACADEMIC/INDUSTRIAL POSITIONS

Nov 2014-present	Professor, Jawaharlal Nehru University
Jan-Mar, 2020	Visiting Scientist, Stony Brook University
May-Oct, 2019	Visiting Scientist, University of Oklahoma
Aug 2007-2014	Associate Professor, Jawaharlal Nehru University
Aug-Oct 2008	Visiting Associate Professor, University of California, San Francisco
2004-2007	Assistant Professor, Indian Institute of Technology, Guwahati, India
2003	Post-Doctoral Fellow, Lawrence Berkeley National Laboratory
Sep-Dec, 2002	Scientist at ARQULE INC., Redwood City, California

EDUCATION/TRAINING

Institution	Degree	Year(s)	Field
Indian Institute of Technology, Kanpur	M.Sc.	1994	Chemistry
Graduate University for Advanced Studies, Japan	Ph.D.	1999	Theoretical and Computational Chemistry
Iowa State University	Post-Doc	1999-2001	Theoretical and Computational Chemistry
University of California, San Francisco	Post-Doc	2001-2002	Computational Biochemistry and Biophysics

RESEARCH ACHIEVEMENTS:

Advancement of several computer simulation algorithms/methods:

- Published several papers on a nested Monte Carlo technique that can increase the speed of computer simulation by orders of magnitude for both quantum mechanical/molecular mechanical (QM/MM) and classical systems
- Developed a new method to explore the energy surface of complex molecules known as Monte Carlo Temperature Basin Paving (MCTBP)
- In collaboration with Prof. Ken Dill, developing a fast and accurate solvation model for MD simulation of biomolecules to significantly increase the applicability of MD simulation

State-of-the-art applications to biological systems:

- Diffusion of proteins in a full *E. coli* cell
- Accurate binding free energy calculations for designing the active sites of calcium-binding proteins
- Innovative calculations of protein-protein binding affinities in solutions with high salt concentrations

FELLOWSHIPS, HONORS AND AWARDS:

- Distinguished Lecture award from the Chemical Society of Japan, 2013

- Finalist for the Swarnajayanti Award in chemistry (An award to recognize scientists below 40 years old in India), 2009
- Indo-US research fellowship to conduct research at the University of California, San Francisco, 2008.
- Monbusho (Japanese Government) scholarship for foreign graduate students, 1996-1999
- Best Masters project award in chemistry from the Indian Institute of Technology, Kanpur, 1994

CURRENT GRANTS:

- Toward manipulation of the binding affinity of a calcium (Ca^{2+}) ion to calcium-binding proteins using computational approaches with experimental validations; with Co-PI Prof. S. Gourinath; from the Department of Biotechnology of India.
- Path towards an ultrafast model of solvation of molecules and its connection to complex processes in biology; with Prof. T. Urbic of University of Lubjijana, Slovenia; Indo-Slovenia Bilateral Grant
- Development of an analytical model of solvation in water using statistical mechanics; Mathematical Research Impact Centric Support (MATRICS), India

PERSONNEL TRAINED:

• 7 PhD students awarded degrees; • 5 current Ph.D. students: • 2 Post-Doctoral Fellows; • 15 Master's Students

SELECTED INVITED LECTURES AND MEETING SESSIONS CHAIRED:

Aug 2023	WATER MEETING, Stony Brook University
Feb 2023	APACC, Vietnam
2022	Theoretical Chemistry Symposium, IISER Kolkata, India
2019	University of Texas, Austin
2019	PNNL, USA
2017	Rare Event Simulation, Agra, India
2017	Energy Landscape meeting, Goa,
2010	Telluride Meeting on Energy Landscapes,

TEACHING EXPERIENCE:

Multiple Undergraduate, Masters and Doctorate level courses in the last 19 years including:

• Biomolecular simulation, • Computational Structural Biology, • Basic Thermodynamic and Statistical Mechanics, • Statistical Mechanics for Biomolecules, • Advances in Physical Science, • Basic Quantum Chemistry

COURSES DESIGNED:

• Biomolecular simulation, • Statistical Mechanics for Biomolecules

MAJOR ADMINISTRATIVE COMMITTEES

- Chair, The Graduate Advisory Committee
- Spearheaded the introduction of a regular Ph.D. course in our school in 2009
- Faculty recruitment committee

OTHER PROFESSIONAL SERVICE:

• Organized 2 International conferences in 2011 and 2013; • Ph.D. Thesis reviewer of top Indian institutes and universities such Indian Institute of Science, and different IITs. • Peer reviewer for J Chem

Phys, JPhysChem, JBiolStrdyn, Biophys J, ACS Omega, ChemPhysLett; • Selection Committee member for the faculty member recruitment in another university.

SELECTED PUBLICATIONS

For the full list see Pradipta Bandyopadhyay - Google Scholar

1. Srivastava, R.; Bandyopadhyay, P. Nested Monte Carlo Simulation of Ionic Systems with the Primitive Model Using Debye-Hückel (DH) Potential as an Importance Function and Optimizing the DH Potential with Kullback-Leibler Divergence Minimization. ***J. Chem. Sci.*** **2023**, *135* (2). https://doi.org/10.1007/s12039-023-02167-0.
2. Roy, U. C.; Bandyopadhyay, P. Correlation between Protein Conformations and Water Structure and Thermodynamics at High Pressure: A Molecular Dynamics Study of the Bovine Pancreatic Trypsin Inhibitor (BPTI) Protein. ***J. Chem. Phys.*** **2023**, *158* (9). https://doi.org/10.1063/5.0124837.
3. Yadav, A. K.; Bandyopadhyay, P.; Coutsias, E. A.; Dill, K. A. Crustwater: Modeling Hydrophobic Solvation. ***J. Phys. Chem. B*** **2022**, *126* (32), 6052–6062. https://doi.org/10.1021/acs.jpcb.2c02695.
4. Basit, A.; Yadav, A. K.; Bandyopadhyay, P. Calcium Ion Binding to the Mutants of Calmodulin: A Structure-Based Computational Predictive Model of Binding Affinity Using a Charge Scaling Approach in Molecular Dynamics Simulation. ***J. Chem. Inf. Model.*** **2022**, *62* (11), 2821–2834. https://doi.org/10.1021/acs.jcim.2c00428.
5. Srivastava, R.; Chattopadhyaya, M.; Bandyopadhyay, P. Calculation of Salt-Dependent Free Energy of Binding of β-Lactoglobulin Homodimer Formation and Mechanism of Dimer Formation Using Molecular Dynamics Simulation and Three-Dimensional Reference Interaction Site Model (3D-RISM): Diffuse Salt Ions and Non-Polar Interactions between the Monomers Favor the Dimer Formation. ***Phys. Chem. Chem. Phys.*** **2020**, *22* (4), 2142–2156. https://doi.org/10.1039/c9cp05578a.
6. Rakshit, A.; Bandyopadhyay, P.; Heindel, J. P.; Xantheas, S. S. Atlas of Putative Minima and Low-Lying Energy Networks of Water Clusters n = 3-25. ***J. Chem. Phys.*** **2019**, *151* (21). https://doi.org/10.1063/1.5128378.
7. Singh, P.; Sarkar, S. K.; Bandyopadhyay, P. Folding-Unfolding Transition in the Mini-Protein Villin Headpiece (HP35): An Equilibrium Study Using the Wang-Landau Algorithm. ***Chem. Phys.*** **2016**, *468*, 1–8. https://doi.org/10.1016/j.chemphys.2016.01.005.
8. Hasnain, S.; Bandyopadhyay, P. An Analytical Correlated Random Walk Model and Its Application to Understand Subdiffusion in Crowded Environment. ***J. Chem. Phys.*** **2015**, *143* (11). https://doi.org/10.1063/1.4930275.
9. Hasnain, S.; McClendon, C. L.; Hsu, M. T.; Jacobson, M. P.; Bandyopadhyay, P. A New Coarse-Grained Model for E. Coli Cytoplasm: Accurate Calculation of the Diffusion Coefficient of Proteins and Observation of Anomalous Diffusion. ***PLoS One*** **2014**, *9* (9). https://doi.org/10.1371/journal.pone.0106466.
10. Bandyopadhyay, P. Increasing the Efficiency of Monte Carlo Simulation with Sampling from an Approximate Potential. ***Chem. Phys. Lett.*** **2013**, *556*, 341–345. https://doi.org/10.1016/j.cplett.2012.11.047.
11. Bandyopadhyay, P.; Kuntz, I. D. Computational Investigation of Kinetics of Cross-Linking Reactions in Proteins: Importance in Structure Prediction. ***Biopolymers*** **2009**, *91* (1), 68–77. https://doi.org/10.1002/bip.21083.
12. Bandyopadhyay, P. Accelerating Quantum Mechanical/Molecular Mechanical Sampling Using Pure Molecular Mechanical Potential as an Importance Function: The Case of Effective Fragment Potential. ***J. Chem. Phys.*** **2005**, *122* (9). https://doi.org/10.1063/1.1861890.