Curriculum Vitae

1. **Name:** **Designation:** **Institution and address:**	**SRABANI TARAPHDER** (*nee′* Roy) Professor Department of Chemistry Indian Institute of Technology Kharagpur 721302 India E-mail: srabani@chem.iitkgp.ernet.in FAX: +91-3222-255303 Telephone: +91-3222-283336 (office) 283853 (residence) 280853 (- do-) Web site : http://www.chemistry.iitkgp.ac.in/~srabani/
2. **Date of birth**	31st July, 1969
3. **Place of birth**	Calcutta, India
4. **Nationality**	Indian
5. **Marital status**	Married
6. **Educational qualification:** (a) B. Sc. in Chemistry (Hons.) (b) M.S. in Chemistry (c) Ph.D. in Physical Chemistry A. Thesis research for Ph.D.: B. Thesis supervisor:	 Presidency College, Calcutta University, Calcutta, India – 1990 Indian Institute of Science, Bangalore, India - 1992 Indian Institute of Science, Bangalore, India – 1996 ***Molecular Relaxation in Liquids : From Ultrafast to Ultraslow Dynamics in Dipolar Solvents*** Professor Biman Bagchi Solid State and Structural Chemistry Unit Indian Institute of Science, Bangalore, India.

7. **Professional Experience:**

- Visiting fellow, Harischandra Research Institute (Formerly known as the Mehta Research Institute of Mathematics and Mathematical Physics) Allahabad, India: Nov. 1995-Oct. 1996.
- Visiting Scientist, Institute of Physics, Bhubaneswar, India: June-July 1996
- Visiting Lecturer, Department of Chemistry, Indian Institute of Technology, Kharagpur, India: Nov. 1996-Feb. 1998.
- Assistant Professor, Department of Chemistry, Indian Institute of Technology, Kharagpur, India: Feb. 1998-Apr.2007.
- Associate Professor, Department of Chemistry, Indian Institute of Technology, Kharagpur, India: Apr.2007-Nov.2011.
- Professor, Department of Chemistry, Indian Institute of Technology, Kharagpur, India: Nov. 2011 – present.
- Category A speaker, Theoretical Physics Seminar Circuit Programme, 1995-1996. Delivered lectures at Institute of Physics, Bhubaneswar, Indian Association for Cultivation of Science, Calcutta, Indian Institute of Technology, Kanpur and Mehta Research Institute, Allahabad.
- Category B speaker, Theoretical Physics Seminar Circuit Programme, 2003-2004.
- Visiting Scientist, Department of Chemistry, University of Chicago, USA: May 1997.
- Visiting Scientist, Laboratoire de Physique Theorique des Liquides, Universite Pierre et Marie Curie, Paris, France: May 1997
- Visiting Fellow, Laboratory of Chemical Physics, National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health, USA: June 2000-July 2001
- Visiting Scientist, Department of Physics, Michigan State University, USA: April 2000.
- Visiting Scientist, Department of Theoretical Physics, University of Trieste, Italy: July 2002.
- Visiting Scientist under Junior Associateship scheme, International Centre for Theoretical Physics, Trieste, Italy: June-July, 2003.
- Short term fellow of the Human Frontier Sciences Program to Instituto de Quimica Fisica Rocasolano, CSIC, Madrid, Spain: June-August 2004.
- Visiting Scientist, Tata Institute for Fundamental Research, Mumbai, India: December 2004.
- Visiting scientist, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany: May 2005.
- Visiting Scientist under Regular Associateship scheme, International Centre for Theoretical Physics, Trieste, Italy: April, 2007.
- Visiting Scientist, Department of Biophysics and of Biochemistry, Albert Einstein College of Medicine of the Yeshiva University, New York, USA: May, 2008.
- Invited lecture, Department of Computer and Information Science, Indiana University-Purdue University, Indianapolis, USA: May 2008.
- Invited lecture, Laboratory of Chemical Physics, National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health, USA: May 2008.

- IUSSTF fellow and visiting scientist, Henry Eyring Center for Theoretical Chemistry, Department of Chemistry, University of Utah, USA: August 2009 – July 2010.
- Visiting Scientist, Department of Chemical Engineering, Colorado School of Mines, USA: June 2011.

8. **Conferences/Workshops attended from 1997:**

- Participant in *Spring Colleges in Computational Physics: College on Molecular Dynamics Simulation*, International Centre for Theoretical Physics, Trieste, Italy: June 1997.
- Participant in *Adriatico Research Conference on Simple Systems at High Temperature and Pressure: Theory and Experiment*, International Centre for Theoretical Physics, Trieste, Italy: July 1997.
- Invited speaker, *Seminar on Some Aspects of Structure, Functionality and Reactivity in Chemistry*, Presidency College, Kolkata: December 1997.
- Invited speaker, *International Conference on Electronic Structure and Dynamics*, Indian Association for Cultivation of Science, Calcutta: January 1998.
- Presentation of poster in *Discussion Meeting on Ultrafast Chemical Phenomena*, Indian Institute of Science, Bangalore: March 1998.
- Participant in *Spring College on Statistical Mechanics and Dynamics of Soft Condensed Matter*, International Centre for Theoretical Physics, Trieste, Italy: May-June, 1998.
- Participant in *Adriatico Research Conference on Complex Systems Far from Equilibrium*, International Centre for Theoretical Physics, Trieste, Italy: June 1998.
- Invited speaker, *Winter School on Statistical Mechanics and Computer Simulation Techniques in Chemistry*, Indian Institute of Technology, Kanpur: February 2000.
- Participant, *Proton Transport in Liquids, Solids and Proteins, 220th National ACS Meeting*, Washington DC, USA: August 2000.
- Invited speaker, *Discussion Meeting On Condensed Matter Physics*, Indian Institute of Technology, Kharagpur: December 2001.
- Invited speaker, *Statphys-Kolkata IV*, Indian Association for Cultivation of Science, Calcutta: January 2002.
- Invited speaker, *National Conference on Recent Trends in Biology Inspired Physics*, S.N. Bose National Centre for Basic Sciences, Calcutta: March 2002
- Invited speaker, *13th Mid-year meeting of the Indian Academy of Sciences*, Bangalore: July 2002
- Poster presentation (*in absentia*), *Fifth Liquid Matter Conference of The European Physical Society*, University of Konstanz, Germany: September 2002.
- Invited speaker, *Trends in Theoretical Chemistry 2002*, Indian Association for Cultivation of Science, Calcutta: January 2003.
- Poster presentation (*in absentia*), *Gordon Conference on Protons and Membrane Reactions*, Ventura, California, USA: February 2003.
- Invited speaker, *One day Symposium on Physics at the Interface of Chemistry*, S. N. Bose National Centre for Basic Sciences, Kolkata: December 2003.
- Invited participant, *Indo-Japan Workshop on Frontiers of Molecular Science Developed by Advanced Spectroscopy*, Indian Association for the Cultivation of Science, Kolkata, India: December 2004.

- Invited speaker, *Symposium on Theoretical Chemistry*, Bhabha Atomic Research Centre, Mumbai, India: December 2004.
- Speaker, *CECAM workshop on Simulation of rare events: The reaction coordinate problem in complex systems*, Centre Européen de Calcul Atomique et Moléculaire (CECAM), Lyon, France: June 2005.
- Speaker, *International Workshop on Classical and Quantum Dynamical Simulations in Chemical and Biological Physics*, Max Planck Institute for Physics of Complex Systems, Dresden, Germany: June 2005.
- Abstract accepted for presentation, Gordon Research Conference on Computational Chemistry 2006, held at Les Diablerets Conference Center, Les Diablerets, Switzerland: October (2006).
- Invited speaker, *DAE-BRNS Theme Meeting on Materials Modeling at Different Length Scales (MMM-2006)*, Bhabha Atomic Research Centre, Mumbai, India: October 2006.
- Invited speaker, *One-day Symposium on Theoretical Chemistry*, Centre for Theoretical Studies, Indian Institute of Technology, Kharagpur: March, 2007.
- Participant and poster presentation, Spring College on '*Water in Physics, Chemistry and Biology*', International Centre for Theoretical Physics, Trieste, Italy: April 2007.
- Invited speaker, *4th IFLASC meeting of the Joint Indo-French Laboratory*, Solid State & Structural Chemistry Unit, Indian Institute of Science, Bangalore, India: June 2007.
- Invited speaker, *Workshop on Structure & Dynamics of Biomolecules-2007*, S.N. Bose National Centre for Basic Sciences, Kolkata: December 2007.
- Invited speaker, Conference on Protein Dynamics and Catalysis, Albert Einstein College of Medicine of the Yeshiva University, New York, USA: May 2008.
- Invited speaker, *Discussion Meeting on Theoretical Chemistry (TCS-2009)*, Indian Institute of Science and JNCASR, Bangalore, India: January 2009.
- Invited speaker, *Frontiers in Chemical Biology: Proteins Structure, Function & Dynamics*, Indian Institute of Science and JNCASR, Bangalore, India: July 2009.
- Session Chair, *Theoretical Chemistry Symposium* (*TCS-10*), Indian Institute of Technology, Kanpur, India: December 2010.
- Invited speaker, *International Symposium on Chemistry & Complexity*, Indian Association for the Cultivation of Science, Kolkata, India: December 2011.
- Invited Speaker, *National Seminar on Current Trends in Chemistry VI* (NSCTC-VI), Kalyani University, India: March 2012.
- Invited Speaker, *Recent Trends in Chemical Science and Technology* (RTCST-2012), IIT Patna, India: March, 2012.
- Invited Speaker, *Theoretical Chemistry Symposium* (*TCS-12*), Indian Institute of Technology, Guwahati, India: December 2012.
- Invited Speaker, *Indo-US Research Conclave,* hosted by IUSSTF, Pune, India: March, 2013.
- Invited Speaker, DAE BRNS Symposium on *Current Trends in Theoretical Chemistry* (CTTC-2013), Bhabha Atomic Research Centre, Mumbai: September 2013.
- Invited Speaker, Telluride Science Research Center Workshop on *Protein Dynamics*, Telluride, CO, USA: August 2013.
- Invited Speaker, *Dynamics of Complex Chemical and Biological Systems,* Indian Institute of Technology, Kanpur, India: February 2014.

- Invited Speaker, *Recent Advances in Modeling Rare Events (RARE2014)*, hosted by Indian Institute of Technology, Kanpur at Alappuzha (Kerala), India: May 2014.
- Invited Speaker, Symposium on Advances in Spectroscopy and Ultrafast Dynamics, Indian Association for the Cultivation of Science, Kolkata, India: December 2014.
- Session Chair, 14th Theoretical Chemistry Symposium, NCL, Pune, India: December 2014.
- Invited Speaker, "Frontiers in Chemistry 2015" at University of North Bengal, India: February 2015.
- Speaker, CECAM Workshop: 'From trajectories to reaction coordinates: making sense of molecular simulation data', held at the Erwin Schrodinger International Institute for Mathematical Physics (ESI), University of Vienna, Austria: September 2015.
- Participant, Free Energy Calculation and Molecular Kinetics Workshop, King's College, London, UK: September 2016.
- Invited talk, CANES (Cross-Disciplinary Approaches to Non-Equilibrium Systems) seminar series, King's College, London, UK: September 2016.
- Participant and Poster presentation, Faraday Discussion on Rate Reaction Theory, organized by the Royal Society of Chemistry, University of Cambridge, Cambridge, UK: September 2016.
- Invited Speaker, Fifteenth Theoretical Chemistry Symposium (TCS 2016), University of Hyderabad, India: December 2016.
- Invited Speaker, International Symposium on Recent Advances in Modeling Rare Events, Agra, India *(RARE2017)*, hosted by Indian Institute of Technology, Kanpur at Agra, India: December 2017.
- Invited Speaker, New perspective to Advanced Functional Materials (NPAFM 2017), Ravenshaw University, Cuttack, Odisha, India: December 2017.
- Invited Speaker, National Symposium on Contributions of Women in Science in India (NSCWSI-2018), Calcutta University, Kolkata, India: February 2018.
- Invited lecture, at the Department of Chemistry, National Institute of Meghalaya, Shillong, India: March 2018.
- Invited lecture, National Seminar on Current Trends in Chemistry VIII, Kalyani University, India: March 2018.
- Speaker, conference on "Computational Chemistry Meets Artificial Intelligence" EPFL, Lausanne, Switzerland: June 2018.
- Invited lecture, Conference on Recent Advances in "Dynamics at the Interface of Chemistry and Biology" (DICB-2019), Indian Institute of Science, Bangalore, India: February 2019.
- Invited lecture, Workshop cum Symposium on Advanced Simulation Methods: DFT, MD and Beyond (ASM2019) Indian Institute of Technology, Delhi, India: March 2019.
- Invited lecture, Workshop on "Free Energy Calculations for Chemical and Biological Systems", Indian Institute of Technology, Kanpur, India: March 2019.

9. **Ranks and Award:**

- Ranked first in the Secondary Examination, West Bengal Board of Secondary Education: 1985.
- National Merit Certificate: 1985.

- Ranked tenth in Higher Secondary Examination, West Bengal Council for Higher Secondary Education: 1987.
- Ranked second in Chemistry (Hons.), Calcutta University: 1990.
- Best poster award in *Trombay Symposium on Radiation and Photochemistry*, Bhabha Atomic Research Centre, Trombay: January 1994.
- Best speaker award in *Unit Day Symposium of Solid State and Structural Chemistry Unit*, Indian Institute of Science, Bangalore: November 1994.
- Elected Junior Associate of the International Centre for Theoretical Physics, Trieste, Italy: 1999-2004 (Extended upto 2005).
- Elected Young Associate of the Indian Academy of Sciences, Bangalore: 1999-2004.
- Short-term fellowship award, Human Frontier Sciences Program, France: 2004
- Elected Regular Associate of the International Centre for Theoretical Physics, Trieste, Italy: 2006-2011.
- Publication in J. Phys. Chem. B, **112**, 13597 (2008) *highlighted in Nature India, Oct. 2008, doi:10.1038/nindia.2008.301*
- Awarded the Indo-US Research Fellowship 2009 by the Indo-US Science & Technology Forum.
- Affiliate member (by invitation), Royal Society of Chemistry, UK: 2017.
- INSA Teachers Award (2018), Indian National Science Academy, New Delhi, India.

10. **Research Interests:**

Theoretical and computer simulation studies related to dynamics in condensed phases and chemical reaction dynamics in solutions and complex biological systems including:

- Conformational fluctuations in biological systems like proteins
- Quantum-mechanical molecular mechanical simulations of elementary chemical reactions
- Development of reaction coordinates of enzyme catalyzed reactions
- Rare event simulation to obtain free energy and rates of chemical reactions
- Molecular modeling of functionalized carbon nanotubes.

11. **List of Journal Publications:**

1. Ultrafast Underdamped Solvation: Agreement Between Computer Simulations And Various Theories Of Solvation Dynamics, **Srabani Roy** and Biman Bagchi, J. Chem. Phys. **99**, 1310-1319 (1993).
2. Molecular Theory Of Ultrafast Solvation In Liquid Acetonitrile, **Srabani Roy**, Snehasudha Komath and Biman Bagchi, J. Chem. Phys. (*Rapid Communications*), **99**, 3139 (1993).
3. Solvation Dynamics In Liquid Water - A Novel Interplay Between Librational And Diffusive Modes, **Srabani Roy** and Biman Bagchi, J. Chem. Phys. **99**, 9938 (1993).
4. Ultrafast Solvation from Kerr Relaxation and Far-Infrared Spectroscopy in Underdamped Dipolar Liquids, Biman Bagchi and **Srabani Roy**, in *Ultrafast Chemical Reactions and Solvent Effects*, Ed. Y. Gauduel and P. J. Rossky (American Institute of Physics, New York, 1993), p. 296.

5. Dielectric Friction and Solvation Dynamics - Novel Results on Relaxation in Dipolar Liquids, **Srabani Roy**, Snehasudha Komath and Biman Bagchi, Proc. Indian Acad. Sci. (Chem. Sci.) (*Rapid Communication*), **105**, 79-85 (1993).
6. Molecular Theory of Ion Solvation Dynamics in Water, Acetonitrile and methanol - A Unified Microscopic Description of Collective Dynamics in Dipolar Liquids, **Srabani Roy** and Biman Bagchi, Proc. Indian Acad. Sci. (Chem. Sci.), **105**, 295-301 (1993).
7. Solvation Dynamics, Energy-Distribution and Trapping of a Light Solute Ion, **Srabani Roy** and Biman Bagchi, Chem. Phys. **183**, 207-216 (1994).
8. Time-Dependent Solution of Generalized Zusman Model of Outersphere Electron-Transfer Reactions - Applications to Various Experimental Situations, **Srabani Roy** and Biman Bagchi, J. Chem. Phys. **100**, 8802-8816 (1994).
9. Microscopic Theory of Ion Solvation Dynamics in Liquid Methanol, **Srabani Roy** and Biman Bagchi, J. Chem. Phys. **101,** 4150-4155 (1994).
10. Effects of Ultrafast Solvation on The Rate of Adiabatic Outer- Sphere Electron-Transfer Reactions, **Srabani Roy** and Biman Bagchi, J. Phys. Chem. **98**, 9207-9215 (1994).
11. Ultrafast Solvation Dynamics in Water - Isotope Effects and Comparison with Experimental Results, Nilashis Nandi, **Srabani Roy** and Biman Bagchi, J. Chem. Phys. **102**, 1390-1397 (1994).
12. Dielectric Relaxation in Dipolar Solid Rotator Phases, G. V. Vijayadamodar, Snehasudha Komath, **Srabani Roy** and Biman Bagchi, Phase Transitions, **50**, 21 (1994).
13. Effects of Solvent Polarization Relaxation on Nonadiabatic Outersphere Electron Transfer Reactions in Ultrafast Dipolar Solvents, **Srabani Roy** and Biman Bagchi, J. Chem. Phys. **102**, 7937-7944 (1995).
14. Adiabatic and Nonadiabatic Outersphere Electron Transfer Reactions in Methanol - Effects of the Ultrafast Solvent Polarization Modes, **Srabani Roy** and Biman Bagchi, J. Chem. Phys. **102**, 6719-6726 (1995).
15. Collective Effects on Single-Particle Orientational Relaxation in Slow Dipolar Liquids, S. Ravichandran, **Srabani Roy** and Biman Bagchi, J. Phys. Chem. **99**, 2489-2501 (1995).
16. Ionic And Dipolar Solvation Dynamics in Liquid Water, Nilashis Nandi, **Srabani Roy** and Biman Bagchi, Proc. Indian Acad. Sci. (Chem. Sci.), **106**, 1297-1306 (1995).
17. Anomalous Ion Diffusion in Dense Dipolar Liquids, Ranjit Biswas, **Srabani Roy** and Biman Bagchi, Phys. Rev. Lett. 75, 1098-1101 (1995). [*Erratum: ibid*, **76**, 556 (1996).]
18. A Molecular Theory for the Rank Dependence of Orientational Relaxation in Brownian Dipolar Lattice, **Srabani Taraphder**, J. Chem. Phys. **109**, 4948-4959 (1998).
19. Dynamic Proton Transfer Pathways in Proteins: Role of Sidechain Conformational Fluctuations, **Srabani Taraphder** and Gerhard Hummer, Physica A, **318,** 293-301 (2003).
20. Protein Side-Chain Motion and Hydration in Proton Transfer Pathways. Results for Cytochrome P450cam, **Srabani Taraphder** and Gerhard Hummer, J. Am. Chem. Soc. **125**, 3931-3940 (2003).
21. Fluid Phase Diagrams of Binary Mixtures from Constant Pressure Integral Equations, Giorgio Pastore, Robert Santin, **Srabani Taraphder** and F. Colonna, J. Chem. Phys. **122**, Art. No. 181104 (2005).

22. Molecular Dynamics Study of the Density and Temperature Dependence of Bridge Functions in Normal and Supercritical Lennard-Jones Fluids, Tapas R. Kunor and **Srabani Taraphder**, Phys. Rev. E, **72**, 031201 (2005)
23. Proton Transfer Pathways in the Mutant His-64–Ala of Human Carbonic Anhydrase II, Arijit Roy and **Srabani Taraphder**, Biopolymers, **82**, 623 (2006) [***Cover page article***].
24. Bridge Functions near the Liquid-vapor Coexistence Curve in Binary Lennard-Jones Mixtures, Tapas R. Kunor and **Srabani Taraphder**, Phys. Rev. E **74**, 011201 (2006).
25. Equilibrium Correlations and Thermodynamics in Low Density Supercritical Lennard-Jones Fluids, Tapas R. Kunor and **Srabani Taraphder**, Physica A, **383**, 401 (2007).
26. Effect of Electrostatic Interactions on the Formation of Proton transfer pathways in Human Carbonic Anhydrase II, Arijit Roy and **Srabani Taraphder**, J. Chem. Sci. (Special Issue), **119**, 545 (2007).
27. Identification of Proton-Transfer Pathways in Human Carbonic Anhydrase II, Arijit Roy and **Srabani Taraphder**, J. Phys. Chem. B, **111**, 10563-10576 (2007).
28. A Theoretical Study on the Detection of Proton Transfer Pathways in Some Mutants of Human Carbonic Anhydrase II, Arijit Roy and **Srabani Taraphder**, J. Phys. Chem. B, **112**, 13597-13607 (2008) [***Highlighted research article in Nature India, Oct. 2008, doi:10.1038/nindia.2008.301***].
29. Free energies of supercritical solvation from molecular dynamics simulation and integral equation studies, Tapas R. Kunor and **Srabani Taraphder**, Physica A, **388**, 1491-1499 (2009).
30. Proton Affinities of Some Amino Acid Side Chains in a Restricted Environment, T.G. Abi, Amit Anand and **Srabani Taraphder,** J. Phys. Chem. B. **113**, 9570-9576 (2009).
31. Transition Path Sampling Study of the Conformational Fluctuation of His-64 in Human Carbonic Anhydrase II, Arijit Roy and **Srabani Taraphder**, J. Phys. Chem. B. **113**, 12555-12564 (2009).
32. Role of Protein Motions on Proton Transfer Pathways in Human Carbonic Anhydrase II, Arijit Roy and Srabani Taraphder, Biochim. Biophys. Acta Proteins & Proteomics, *Special issue on Carbonic Anhydrase and Superoxide Dismutase*, **1804**, 351-361 (2010). [*invited article*]
33. Chemical Rescue of Enzymes: Proton Transfer in Mutants of Human Carbonic Anhydrase II, C. Mark Maupin, Norberto Castillo, **Srabani Taraphder**, Chingkuang Tu, Robert McKenna, David N. Silverman and Gregory A. Voth, J. Am. Chem. Soc. **133**, 6223-6234 (2011).
34. Understanding Proton Affinity of Tyrosine Sidechain in Hydrophobic Confinement, T. G. Abi, Tarak Karmakar and **Srabani Taraphder**, *Invited article,* J. Chem. Sci. (Special Issue), **124**, 59-63 (2012).
35. Proton Transfer Reactions in Carbon Nanotubes Endohedrally Functionalized with Selected Polar Amino Acid Sidechains, T. G. Abi and **Srabani Taraphder**, Chem. Phys. **405**, 107-116 (2012).
36. Modeling the Structure and Proton Transfer Pathways of the Mutant His-107-Tyr of Human Carbonic Anhydrase II, Puspita Halder and **Srabani Taraphder,** J. Mol. Model. **19**, 289-198 (2013).
37. Proton Affinity of Polar Amino Acid Sidechain Analogues Anchored to the Outer Wall of Single Walled Carbon Nanotubes, T. G. Abi, Tarak Karmakar and Srabani Taraphder, Computational and Theoretical Chemistry, **1010**, 53-66 (2013).

38. Free Energies of Proton Transfer by Polar Amino Acid Sidechain Analogues Anchored to the Outer Wall of Single Walled Carbon Nanotubes, T. G. Abi and Srabani Taraphder, Computational and Theoretical Chemistry, **1027**, 19-25 (2014).
39. Structure and Dynamics of Water inside Endohedrally Functionalized Carbon Nanotubes, Sanjib Paul, T. G. Abi and Srabani Taraphder, J. Chem. Phys. **140**, 184511 (2014).
40. Determination of the Reaction Coordinate for a Key Conformational Fluctuation in Human Carbonic Anhydrase II, J. Phys. Chem. *invited article for Biman Bagchi Festschrift*, **119**, 11403-11415 (2015).
41. Identification of Putative Unfolding Intermediates of the Mutant His-107-Tyr of Human Carbonic Anhydrase II in a Multidimensional Property Space, Puspita Halder and **Srabani Taraphder**, Proteins Structure Function & Bioinformatics, **84**, 726-743 (2016).
42. Coupling Protein Dynamics with Proton Transport in Human Carbonic Anhydrase II, **Srabani Taraphder**, C. Mark Maupin, Jessica M. J. Swanson, and Gregory A. Voth, J. Phys. Chem. B, **120**, 8389-8404 (2016).
43. Functionalized single walled carbon nanotubes as template for water storage device, Sanjib Paul and **Srabani Taraphder**, Chem. Phys. **479**, 42-52 (2016).
44. Small Nonplanar Phenothiazine-5-oxide-Based Molecules: Structural Characterization, Photophysical, Thermal and Computational Studies, Swati Bishnoi, Marilyn Daisy Milton, Tanmoy Kumar Paul, Arun Kumar Pal and **Srabani Taraphder**, ChemistrySelect **2**, 3084 – 3092 (2017).
45. Unfolding intermediates of the mutant His-107-Tyr of human carbonic anhydrase II, **Srabani Taraphder**, Puspita Halder, Tanmoy Kumar Paul and Satyajit Khatua, J. Chem. Sci. (Special Issue on Theoretical Chemistry/Chemical Dynamics (*invited article*) **129**, 1031–1044 (2017).
46. Reaction Coordinate, Free Energy and Rate of Intramolecular Proton Transfer in Human Carbonic Anhydrase II, Sanjib Paul, Tanmoy Kumar Paul and **Srabani Taraphder**, J. Phys. Chem. B **122**, 2851-2866 (2018).
47. Novel Phenothiazine-5-oxide Based Push-Pull Molecules: Synthesis and Fine Tuning of Electronic, Optical and Thermal Properties, Shweta Chaudhary, Madhubani Mukherjee, Tanmoy K. Paul, Swati Bishnoi, **Srabani Taraphder** and Marilyn D. Milton, ChemistrySelect **3**, 5073 – 5081 (2018).
48. Orthogonal Order Parameters to Model the Reaction Coordinate of an Enzyme Catalysed Reaction, Sanjib Paul, Tanmoy Kumar Paul and **Srabani Taraphder**, J. Mol. Graphics Model. 10.1016/j.jmgm.2019.03.023 (in press, 2019).

12. **Manuscript under Review/Preparation:**

- Novel thiazoline-phenothiazine based "push-pull" molecules as fluorescent probes for volatile acid sensing, Shweta Chaudhary, Madhubani Mukherjee, Tanmoy Kumar Paul, **Srabani Taraphder** and Marilyn Milton (2019, submitted)
- Penta-coordination of zinc ion drives the (de)protonation of key water/hydroxide at the active site of HCA II: A QM-MM simulation study, Tanmoy Kumar Paul and **Srabani Taraphder** (2019).
- Mapping out pathways of entry of a small inhibitor molecule into a protein, Satyajit Khatua and **Srabani Taraphder** (2019).

13. **Sponsored Project(s):**

	Title	P.I. & Co-P.I.	Funding agency	Duration
1.	*Theoretical Investigations on the Dynamics of Chemical Reactions in Sub- and Supercritical Water*	Dr. Srabani Taraphder	ISIRD, IIT Kharagpur	1998-2000
2.	*Theoretical Investigations on the Structure and Dynamics of Liquids under Pressure*	Dr. Srabani Taraphder	Department of Science and Technology (DST), India	2003-2006
3.	*Theoretical Modelling of the Role of Hydration in Proton Transfer Processes in Proteins*	Dr. Srabani Taraphder	Council of Scientific & Industrial Research (CSIR), India	2007-2010
4.	*Computer Simulation Studies of Proton Transfer Reactions in Proteins like Carbonic Anhydrase*	Dr. Srabani Taraphder Co-PI: Prof. G.A. Voth University of Utah, USA	Indo-US Science & Technology Forum (IUSSTF), India	2009-2010
5.	*Computer Simulation Studies on the Role of Protein Motions on Enzyme Catalyzed Proton Transfer Reactions*	Dr. Srabani Taraphder	Council of Scientific & Industrial Research (CSIR), India	2011-2014
6	*Inhibition of Enzymes by Small Molecules: Reaction Coordinates, Free Energy and Rates from Computer Simulation Studies*	Dr. Srabani Taraphder	Science and Engineering Board (SERB), India	2019-2022

14. **M. Sc. thesis supervision**:

	Name of student	Year	Thesis title
1.	Subhasis De	1998	*A Theoretical Study on the Effect of Solvent on the Rates of Outersphere Electron Transfer Reaction*
2.	Anurag Kunwar	2002	*Molecular Dynamics Simulation Study of Lennard-Jones Fluids*
3.	Pratik Dhar	2002	*Theoretical Estimation of Solvent Accessible Surface Area of Molecular Clusters and Biological Macromolecules*

4.	Sandip Kumar	2003	*Effect of Structural Fluctuations on the Cavity Distribution in Proteins*
5.	Ghanashyam Roy	2003	*On the Calculation of Rate Constants of Chemical Reactions and Estimation of Solvent Effects on the Rate*
6.	Himanshu Gupta	2004	
7.	Vishal	2005	*Theoretical Calculation of Possible Hydration Sites inside A Protein using PMF Approach* (In progress)
8.	Trina Ghosh Dastidar	2006	*Study of Alternative Hydration Site in a Protein Molecule*
9.	Amit Anand	2007	*Study of Proton Affinities of Polar Amino Acid Residues of Proteins*
10.	Anirban Bhattacharjee	2007	*Molecular Dynamics Simulation of Density Inhomogeneities in Supercritical Water*
11.	Aditi Das	2008	*Structural and Dynamical Behaviour of Water Molecules along Proton Transfer Pathways in Human Carbonic Anhydrase II*
12.	Mohona Sarkar	2008	*A Study on the Conformational Dynamics of His-64 Mediated Proton Pathway in Human Carbonic Anhydrase II*
13.	Chaitanya Ambi	2009	*Proton Affinities of Amino Acids with Uncharged Polar Sidechains inside Carbon Nanotubes*
14.	Poorna Roy	2009	*Investigation of Proton Transfer Pathways in Enzymatic Catalysis*
15.	Tarak Karmakar	2011	*Density Functional Studies on the Proton Affinity of Amino Acid Sidechains attached to Inner and Outer Surfaces of Single Walled Carbon Nanotubes*
16.	Rudranath Sen	2012	*Dynamics of Water in Functionalized Carbon Nanotubes*
17	Bikram Dalal	2013	
18.	K Nandita	2014	*Molecular Dynamics Simulation of TIP3P Water Box Model at 300 K*
19.	Sumana Saha	2014	*Molecular Dynamics Simulation of TIP3P Water Model at 300 K*
20.	M Jayabharath Reddy	2015	*QM/MM Simulations of the reaction between Human Carbonic Anhydrase II and Carbon Dioxide*
21.	Ajay Kumar	2015	*Molecular Dynamics Simulations of Water and Exohedrally Functionalized Single-Walled Carbon Nanotube in Water*
22.	Navatha Komatireddy	2016	*Comparison of the Structure and Function of Different Isozymes of Human Carbonic Anhydrase*
23	Avik Bhattacharjee	2016	*Normal Mode Analysis of Molecular and Biomolecular Systems*
24	Madhubani Mukherjee	2017	*DFT based quantum mechanical calculations on different systems*

15. **Ph.D. thesis supervision**:

No.	Name of student	Status	Title/Topic
1.	Tapas Ranjan Kunor	Completed, 2006	*Theoretical Investigations on the Structure and Thermodynamics of Supercritical Fluids*

2.	Arijit Roy	Completed, July 2009	*Conformational Dynamics and Detection of Proton Transfer Pathways in Human Carbonic Anhydrase II*
3.	T G Abi	Completed, Oct 2011	*Proton Transfer Reactions in Carbon Nanotubes Functionalized with Amino Acid Sidechains*
4.	Puspita Halder	Completed, Jan. 2015	*Thermal Unfolding and Proton Transfer Activity of the Mutant His-107-Tyr of Human Carbonic Anhydrase II*
5.	Sanjib Paul	Completed, May 2018	*Computer Simulation Studies on the Dynamics of Water and Polar Amino Acid Sidechains in Complex Cavities*
6.	Tamoy Kumar Paul	Ongoing	*Hybrid Quantum Mechanical-Molecular Mechanical Simulations of Enzyme Catalysis*
7.	Satyajit Khatua	Ongoing	*Molecular Mechanism of Enzyme Inhibition*
8.	Divya Rai	Ongoing	*Machine Learning in Molecular Dynamics Simulation*

16. **Teaching experience:**

At the Undergraduate Level

Course title	Level	Academic program
Chemistry (Theory and laboratory)	First year	Common coursework for B.Tech., M.Tech and 5-year M.Sc.
Physical Chemistry I	Second year	5 –year Integrated M.Sc. in Chemistry
Chemistry (Theory and laboratory)	Preparatory	Preparatory Course for SC/SCT students

At the Postgraduate Level

Course title	Level	Academic program
Group Theory for Chemists	M.Sc first year -do-	5 –year Integrated M.Sc. in Chemistry, 2-year M.Sc. in Chemistry
Mathematics for Chemists	M.Sc. first year	2-year M.Sc. in Chemistry
Quantum Chemistry	-do-	-do-
Introduction to Computational Chemistry	-do-	-do-
Physical Chemistry Laboratory	M.Sc. first year	2-year M.Sc. in Chemistry
Physical Chemistry Laboratory	Fifth year	5 –year Integrated M.Sc. in Chemistry
Reaction Dynamics and Photochemistry	Fifth year	5 –year Integrated M.Sc. in Chemistry
Statistical Mechanics	Fifth year M.Sc. second year	5 –year Integrated M.Sc. in Chemistry, 2-year M.Sc. in Chemistry
Advanced Computational Chemistry	Fourth year	5 –year Integrated M.Sc. in Chemistry

(Theory and laboratory)		
Molecular Thermodynamics & Kinetics	M.Sc. first year	Joint M.Sc.-Ph.D. program in Chemistry
Advanced Statistical Mechanics/Statistical Mechanics for Chemists	Fifth year, M.Sc. final year & PhD	5 –year Integrated M.Sc. in Chemistry, Joint M.Sc.-Ph.D. program in Chemistry, Ph.D.

17**. Work in Progress:**

- Coupling of protein dynamics and formation of long range proton transfer pathways in proteins.

Proton transport through proteins constitutes an important step in enzymatic catalysis and in biological energy transduction. A generalized method to identify proton transfer pathways in proteins has been developed and we are currently studying the coupling of protein structural and hydration dynamics to the formation of a long range proton path sampled from the solution structure of the protein.

- Determination of the reaction coordinate of enzyme catalyzed reactions from different dynamical pathways of proton transfer in proteins

The evaluation of an overall rate of proton transfer along a detected path requires a quantum mechanical-molecular mechanical description of the charge transfer process to include the effects of actual bond making and bond breaking that take place during the long range transfer. Work is in progress to optimize a single collective variable, labeled as reaction coordinate, from the identified proton transfer trajectories using QM-MM methods interfaced with transition path sampling simulation studies. We are using advanced methods of machine learning for this purpose.

- Free energy changes and rates of key proton transfer steps

The proton transfer pathways detected by the method outlined above are subjected to further analysis by computing the free energy changes along these pathways. We have used the umbrella sampling method to estimate the contribution of free energy when a transient connection is formed between long-lived patches of hydrogen bonded network inside the protein. We are now trying to generalize the calculations to project the free energy along two or more relevant coordinates.

- Probing the structure, dynamics and function of enzymes in the presence of inhibitiors

Our goal is to probe the mechanism of enzyme catalyzed, rate determining proton transfer steps in the presence of different inhibitors using the methodology of reaction coordinates as outlined above.