

CURRICULUM VITAE
Sudeep Bhattacharyay, Ph.D.

Professor of Chemistry
Councilor, Council of Undergraduate Research
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EDUCATION

1997 Ph.D., Chemistry, Indian Association for the Cultivation of Science, Jadavpur University, Jadavpur, India. Advisor: Prof. Muktimoy Chaudhury
1991 M.Sc., Chemistry, Indian Institute of Technology, Kharagpur, India
1989 B.Sc., Chemistry, Indian Institute of Technology, Kharagpur, India

ACADEMIC EXPERIENCE

2022 Fall Professor, Department of Chemistry, University of Wisconsin-Eau Claire (UW-Eau Claire), Eau Claire, WI
2017-2022 Associate Professor, Department of Chemistry, UW-Eau Claire, Eau Claire, WI
2011-2017 Assistant Professor, Department of Chemistry, UW-Eau Claire, Eau Claire, WI
2007-2010 Adjunct Instructor and Research Professor, Department of Chemistry, UW-Eau Claire, Eau Claire, WI
2003-2007 Research Associate, Department of Chemistry, University of Minnesota, Minneapolis, Minnesota
2000-2002 Postdoctoral Associate, Department of Chemistry, Indiana University, Bloomington, Indiana
1998-1999 Postdoctoral Fellow, Department of Chemistry, Simon Fraser University, Burnaby, BC, Canada
1991-1997 Graduate Research Fellow, Indian Association for the Cultivation of Science, India
Thesis: "Studies on Metal Complexes of Sulfur-Nitrogen Chelating Agents"

TEACHING EXPERIENCE

Regular Semester Courses

Biophysical Chemistry
Physical Chemistry 2 (Quantum Chemistry; Computational Chemistry)
Physical Chemistry 2 (Thermodynamics; Kinetics)
Computational Chemistry
General Chemistry

Course-embedded Research

One of my main teaching interests is to foster active learning through discovery-guided projects. In the past few semesters, authentic research projects have been designed and introduced in biophysical and physical chemistry courses, mostly with seniors. These projects are computational and are being carried out using either a remote server or the in-house Blugold Supercomputing Cluster.

Independent Study

Undergraduate students take independent study courses, during which they are tasked to study literature aligned with their project, discuss the hypothesis they are to probe in group meeting, design and conduct experiments, analyze results, writing manuscripts.

GRANTS AND SCHOLARSHIPS

External/Federal Grants

- 2022, National Science Foundation (NSF), Co-PI, \$385,762 of UW-Eau Claire (**awarded**)
“*REU Site: Advancing High-Performance Computing Opportunities in Undergraduate Research at UW-Eau Claire to Meet Challenges of Multidisciplinary Computational Science*”
- 2021, UW – Madison Tommy Thompson Center of Public Leadership, Co-PI with two UW-Eau Claire faculty, one UW-Stout faculty, and one UW-River Falls faculty, \$94,368 (**awarded**)
“*Exploring Policies to Promote High-Performance Computing in Post-Pandemic Undergraduate Education in Wisconsin*”
- 2020, National Institutes of Health (NIH) - AREA, Co-PI, \$397,331 (**awarded**)
“*Exploring the Dynamics of Prolyl-tRNA Synthetases: Towards Developing a Screening Method for Species-Specific Inhibitors*”
- 2019, NSF-MRI, PI, \$350,000 (**awarded**)
“*MRI: Acquisition of a High-Performance Computing Cluster to Enhance the Undergraduate Discovery Experience*”
- 2016, NIH-AREA, Co-PI, \$383,900 (**awarded**)
“*Exploring the Dynamics of Prolyl-tRNA Synthetases: Towards Developing a Screening Method for Species-Specific Inhibitors*”
- 2014, Research Corporation for Science Advancement, PI, \$55,000 (**awarded**)
“*Towards Developing a Computational Inhibitor Screening Method for Quinone Reductase*”

Major Internal Grant

- 2012 UWEC to Blugold Commitment Differential Tuition fund, PI, \$146,000 (**awarded**)
“*A High-Performance Supercomputer Cluster for UW-Eau Claire*”

AWARDS

- 2021 Excellence in Mentoring Research, Scholarship and Creative Activity, UW-Eau Claire
2021 Recognized at Authors' Celebration Event, UW-Eau Claire
2019 1-year Sabbatical in Department of Physical and Analytical Chemistry, Biocomputing Group, University of James I (UJI) “Quantum Mechanical Tunneling in Flavoenzymes,” UW-Eau Claire
2016 Recognized at Authors Celebration Event, UW-Eau Claire
2009 Recognized at Authors Celebration Event, UW-Eau Claire

RESEARCH WITH UNDERGRADUATE STUDENTS

I use experiment, theory, literature review, and advanced computer simulation methods to explore behaviors of molecules in complex chemical environments. I have incorporated modeling and simulation in Chemistry curriculum. In Fall 2021, I began teaching the novel Computational Chemistry course to aid undergraduate research students. I have maintained an active research program after joining the Chemistry department and was able to publish a total of 21 peer-reviewed publications with **103** undergraduate students, who participated in these research studies.

PEER-REVIEWED ARTICLES (*indicates UW-Eau Claire undergraduate student collaborators)

Peer-reviewed article and book chapter on education and curricular modification

1. *Integrating Research into the Curriculum – A Low-cost Strategy for Promoting Undergraduate Research*, S. Hati, and S. Bhattacharyya, in "**Best Practices for Supporting and Expanding Undergraduate Research in Chemistry**", book chapter, American Chemical Society, Eds. Gourley, B. L. and Jones, R. M., 2018, 119-141.
2. *Incorporating Modeling and Simulations in Undergraduate Biophysical Chemistry Course to Promote Understanding of Structure-Dynamics-Function Relationships in Proteins*, S. Hati and S. Bhattacharyya, *Biochem. Mol. Biol. Educ.*, 2016, 44, 140-59. <https://doi.org/10.1002/bmb.20942>
3. *Inter-institutional Resource Sharing in Undergraduate HPC Education: Interviews with University Administrators* Ghosh, A., Kunkel, W., Varghese, A., Ma, Y., Gomes, R., Bhattacharyya, S., Mohr, M., Doss, I. and Hebert, J., *SIGCSE (Proceedings of the 54th ACM Technical Symposium on Computer Science Education V. 1)* 2023, 1, 848-853. <https://doi.org/10.1145/3545945.3569784>

Peer-reviewed articles with undergraduate student collaborators

(* indicates UW-Eau Claire undergraduate student collaborators)

4. *Polyethylene Glycol 20k. Does it Fluoresce?* Laatsch, B.*; Brandt, M.*; Finke, B.*; Fossum, C. J.*; Wackett, M. J.*; Lowater, H.R.*; Narkiewicz-Jodko, A.*; Le, C. J.*; Yang, T., Glowgowski, E. M., Bailey-Hartsel, S.C., Hati, S. and Bhattacharyya, S. *ACS Omega*, 2023, 8, 14208–14218. <https://doi.org/10.1021/acsomega.3c01124>.
5. *Evolution of Stronger SARS-CoV-2 Variants as Revealed Through the Lens of Molecular Dynamics Simulations*, A. J. Wozney*, M. A. Smith*, M. Abdrabbo*, C. M. Birch*, K. A. Cicigoi*, C. C. Dolan*, A. E. L. Gerzema*, A. Hansen*, E. J. Henseler*, B. LaBerge*, C. M. Leavens*, C. N. Le*, A. C. Lindquist*, R. K. Ludwig*, M. G. O'Reilly*, J. H. Reynolds*, B. A. Sherman*, H. W. Sillman*, M. A. Smith*, M. J. Snortheim*, L. M. Svaren*, E. C. Vanderpas*, M. J. Wackett*, M. M. Weiss*, S. Hati, and S. Bhattacharyya, *Protein J.*, 2022, 41, 1-13. <https://doi.org/10.1007/s10930-022-10065-6> (Chem. 406 project)
6. *Pre-existing Oxidative Stress Creates a Docking-Ready Conformation of the SARS-CoV-2 Receptor-Binding Domain*, C. J. Fossum*, B. F. Laatsch*, H. R. Lowater*, A. W. Narkiewicz-Jodko*, L. Lonzarich, S. Hati and S. Bhattacharyya, *ACS Bio & Med Chem Au.*, 2022, 2, 84–93. <https://doi.org/10.1021/acsbiochemau.1c00040>.
7. *Vitamin D and COVID-19: A Review on the Role of Vitamin D in Preventing and Reducing the Severity of COVID-19 Infection*, M. Abdrabbo*, C. M. Birch*, M. K. A. Brandt*, S. J. Coffey*, C. C. Dolan*, H. Dvorak*, A. C. Gehrke*, A. E. L. Gerzema*, A. Hansen*, E. J. Henseler*, A. C. Huelsbeck*, B. LaBerge*, C. M. Leavens*, C. N. Le*, A. C. Lindquist*, R. K. Ludwig*, J. H. Reynolds*, N. J. Severson*, B. A. Sherman*, H. W. Sillman*, M. A. Smith*, M. A. Smith*, M. J. Snortheim*, L. M. Svaren*, E. C. Vanderpas*, M. J. Wackett*, A. J. Wozney*, S. Bhattacharyya, and S. Hati, *Protein Science*, 2021, 30, 2206–2220. <https://doi.org/10.1002/pro.4190>.
8. *Impact of Thiol-Disulfide Balance on the Binding of Covid-19 Spike Protein with Angiotensin Converting Enzyme 2 Receptor*, S. Hati and S. Bhattacharyya, *ACS Omega*, 2020, 5, 16292-16298. <https://doi.org/10.1021/acsomega.0c02125>
9. *Editing Domain Motions Preorganize the Synthetic Active Site of Prolyl-tRNA Synthetase*, Q. H. Hu*, M. T. Williams*, I. Shulgina, C. J. Fossum*, K. M. Weeks*, L. M. Adams*, C. R. Reinhardt*, K. Musier-Forsyth, S. Hati, and S. Bhattacharyya, *ACS Catal.*, 2020, 10, 10229–10242. <https://doi.org/10.1021/acscatal.0c02381>
10. *Effects of Distal Mutations on Prolyl-adenylate Formation of Escherichia coli Prolyl-tRNA Synthetase*, J. Zajac*, H. Anderson*, L. Adams*, D. Wangmo*, S. Suhail*, A. Almen*, L. Berns*, B. Coerber*, L. Dawson*, A. Hunger*, J. Jehn*, J. Johnson*, N. Plack*, S. Strasser*, M. Williams*,

- S. Bhattacharyya, and S. Hati, *Protein J.*, 2020, 39, 542–553. <https://doi.org/10.1007/s10930-020-09910-3>. (Chem. 406 project).
11. *Role of Oxidative Stress on SARS-CoV (SARS) and SARS-CoV-2 (COVID-19) Infection: A Review*, S. Suhail*, J. Zajac*, C. Fossum*, H. Lowater*, C. McCracken*, N. Severson*, B. Laatsch*, A. Narkiewicz-Jodko*, B. Johnson*, J. Liebau*, S. Bhattacharyya, and S. Hati, *Protein J.*, 2020, 39, 644-656. <https://doi.org/10.1007/s10930-020-09935-8>.
 12. *Crowder-Induced Conformational Ensemble Shift in Escherichia coli Prolyl-tRNA Synthetase*, L. M. Adams*, R. J. Andrews*, Q. H. Hu*, H. L. Schmit*, S. Hati, S., and S. Bhattacharyya, *Biophys. J.*, 2019, 117, 1269-1284. <https://doi.org/10.1016/j.bpj.2019.08.033>.
 13. *Cyclic Changes in Active Site Polarization and Dynamics Drive the 'Ping-pong' Kinetics in NRH:Quinone Oxidoreductase 2: An Insight from QM/MM Simulations*, C. R. Reinhardt*, Q. H. Hu*, C. G. Bresnahan*, S. Hati, S. Bhattacharyya, *ACS Catal.*, 2018, 12, 12015-12029. <https://doi.org/10.1021/acscatal.8b04193>.
 14. *Insight into the Kinetics and Thermodynamics of the Hydride Transfer Reactions between Quinones and Lumiflavin: A Density Functional Theory Study*, C. R. Reinhardt*, T. C. Jaglinski*, A. M. Kastenschmidt*, E. H. Song*, A. K. Gross*, A. J. Krause*, J. M. Gollmar*, K. J. Meise*, Z. S. Stenerson*, T. J. Weibel*, A. Dison*, M. R. Finnegan*, D. S. Griesi*, M. D. Heltne*, T. G. Hughes*, C. D. Hunt*, K. A. Jansen*, A. H. Xiong*, S. Hati, and S. Bhattacharyya, *J. Mol. Model.*, 2016, 22, 199-213. <https://doi.org/10.1007/s00894-016-3074-1>.
 15. *Effect of Stacking Interactions on the Thermodynamics and Kinetics of Lumiflavin: A Study with Improved Density Functionals and Density Functional Tight-Binding Protocol*, Bresnahan, C. G.*, C. R. Reinhardt*, T. G. Bartholow*, J. P. Rumpel*, M. A. North*, and S. Bhattacharyya, *J. Phys. Chem. A*, 2015, 119, 172–182.
 16. *Comparison of the intrinsic dynamics of aminoacyl-tRNA synthetases*, N. Warren*, A. Strom*, B. Nicolet*, K. Albin*, J. Albrecht*, B. Bausch*, M. Dobbe*, M. Dudek*, S. Firgens*, C. Fritsche*, A. Gunderson*, J. Heimann*, C. Her*, J. Hurt*, D. Konorev*, M. Lively*, S. Meacham*, V. Rodriguez*, S. Tadayon*, D. Trcka*, Y. Yang*, S. Bhattacharyya, and S. Hati, *Protein J.*, 2014, 33, 184-98.
 17. *Probing the global and local dynamics of aminoacyl-tRNA synthetases using all-atom and coarse-grained simulations*, A. M. Strom*, S. Fehling*, S. Bhattacharyya, S. Hati, *J. Mol. Model.*, 2014, 20, 2245-55.
 18. *Strictly conserved lysine of prolyl-tRNA synthetase editing domain facilitates binding and positioning of misacylated tRNA^{Pro}*, T. G. Bartholow*, B. L. Sanford*, B. Cao*, H. L. Schmit*, J. M. Johnson*, J. Meitzner*, S. Bhattacharyya, K. Musier-Forsyth, and S. Hati, *Biochemistry*, 2014, 53, 1059-68.
 19. *Multiple pathways promote dynamical coupling between catalytic domains in Escherichia coli prolyl-tRNA synthetase*, J. M. Johnson*, B. L. Sanford*, A. M. Strom*, S. N. Tadayon*, B. P. Lehman*, A. M. Zirbes*, S. Bhattacharyya, K. Musier-Forsyth, and S. Hati, *Biochemistry*, 2013, 52, 4399-4412.
 20. *Role of coupled dynamics in the catalytic activity of prokaryotic-like prolyl-tRNA synthetases*, B. Sanford*, B. Cao*, J. M. Johnson*, K. Zimmerman*, A. M. Strom*, R. M. Mueller*, S. Bhattacharyya, K. Musier-Forsyth, S. Hati, *Biochemistry*, 2012, 51, 2146-56.
 21. *Interplay of flavin's redox states and protein dynamics: an insight from QM/MM simulations of dihydronicotinamide riboside quinone oxidoreductase 2* R. M. Mueller*, M. A. North*, C. Yang*, S. Hati, S. Bhattacharyya *J. Phys. Chem. B*, 2011, 115, 3632-3641.
 22. *Improved density functional description of the electrochemistry and structure-property descriptors of substituted flavins*, M. A. North*, S. Bhattacharyya, D. G. Truhlar, *J. Phys. Chem. B*, 2010, 114, 14907–14915.
 23. *Theoretical determination of the redox potentials of NRH:quinone oxidoreductase 2 using quantum mechanical/molecular mechanical simulations*, J. C. Jr. Rauschnot*, C. Yang*, V. Yang*, S. Bhattacharyya, *J. Phys. Chem. B*, 2009, 113, 8149-8157.

24. *Evolutionary basis for the coupled-domain motions in Thermus thermophilus leucyl-tRNA synthetase*, K. Weimer*, B. Shane*, M. Brunetto, S. Bhattacharyya, and S. Hati, **J. Biol. Chem.**, 2009, 284, 10088-10099.

Selected peer-reviewed articles (prior to joining UW-Eau Claire; 18 peer-reviewed publications in total)

25. *Critical role of substrate conformational change in the proton transfer process catalyzed by 4-oxalocrotonate tautomerase*, J. J. Ruiz-Pernia, M. Garcia-Viloca, S. Bhattacharyya, J. Gao, D. G. Truhlar, and I. Tunon, **J. Am. Chem. Soc.**, 2009, 131, 2687-2698.
26. *Combined quantum mechanical and molecular mechanical simulations of one- and two-electron reduction potentials of flavin cofactor in water, medium-chain acyl-CoA dehydrogenase, and cholesterol oxidase*, S. Bhattacharyya, M. T. Stankovich, D. G. Truhlar, and J. Gao, **J. Phys. Chem. A**, 2007, 111, 5729-5742.
27. *Potential of mean force calculation for the proton and hydride transfer reactions catalyzed by medium-chain acyl-CoA dehydrogenase: effect of mutations on enzyme catalysis*, S. Bhattacharyya, S. Ma., M. T. Stankovich, D. G. Truhlar, and J. Gao, **Biochemistry**, 2005, 44, 16549-16562.
28. *Comparative modeling of the phosphatase and kinase domains of protein tyrosine phosphatase and insulin receptor kinase from Drosophila melanogaster (DPTP61fm), and a computational study of their mutual interactions*, S. Hati, S. Bhattacharyya, J. V. Price, and A. S. Tracey, **Biochemistry and Cell Biology** 2002, 80, 225-239.
29. *V(V) Complexes in Enzyme Systems: Aqueous chemistry, inhibition and molecular modelling in inhibitor design*, S. Bhattacharyya and A. S. Tracey, **J. Inorg. Biochem.** 2001, 85, 9-13.
30. *Interactions of N,N-dimethylhydroxamidovanadium(V) with sulfhydryl-containing ligands: V(V) equilibria and the structure of a V(IV) dithiothreitol complex*, S. Bhattacharyya, A. Martinsson, R. Bachelor, F. W. B. Einstein, A. S. Tracey, **Can. J. Chem.** 2001, 79, 938 - 948.
31. *Synthesis, characterization and reactivity of mononuclear O, N-chelated Vanadium-(IV) and (III) complexes of methyl 2-aminocyclopent-1-ene-1-dithiocarboxylate based ligands: reporting a rare type of conformational isomerism*, S. Bhattacharyya, S. Mukhopadhyay, S. Samanta, T. J. R. Weakley, and M. Chaudhury, **Inorg. Chem.** 2002, 41, 2433-2440.
32. *Intra molecular electron transfer in [(BzIm)(LVO)₂O] (H₂L = S-methyl-(2-hydroxy phenyl) methylenedithiocarbazate): A novel (5-oxo) dinuclear oxovanadium(IV/V) compound with a trapped-valence (V₂O₃)³⁺ core*, S. K. Dutta, S. B. Kumar, S. Bhattacharyya, E. R. T. Tiekink, and M. Chaudhury, **Inorg. Chem.** 1997, 36, 4954-4960.

SERVICE AND SYNERGISTIC ACTIVITIES

- Council of Undergraduate Research, *Councilor*, July 2022 – present
- College of Arts and Sciences Curriculum Committee, *Member*, August 2021 – present
- UW-Eau Claire, Equity, Diversity, and Inclusion Strategic Planning Writing Sub-Committee, *Co-lead*, July 2020 – July 2021
- MERCURY, National Computational Chemistry Consortium Faculty Mentor Subcommittee, *Organizer*, July 2020 – December 2021
- UW-Eau Claire, Department of Chemistry and Biochemistry, Equity, Diversity, and Inclusion Committee, *Chair*, August 2020 – present
- UW-Eau Claire, Blugold Supercomputing Cluster, *Principal Coordinator*, 2013 – present
- Proceeding of the National Academy of Science, Journal of Physical Chemistry, Journal of American Chemical Society, Theoretical Chemical Accounts, Journal of Chemical Theory and Computation, Journal of Molecular Modeling, and International Journal of Quantum Chemistry, Journal of Medicinal Chemistry, *Reviewer*