

CURRICULUM VITAE

Sudeep Bhattacharyay, Ph.D.

Associate Professor of Chemistry

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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

- 2017-present Associate Professor, Department of Chemistry, University of Wisconsin-Eau Claire, Eau Claire, WI 54702, WI
- 2011- 2017 Assistant Professor, Department of Chemistry, University of Wisconsin-Eau Claire, Eau Claire, WI
- 2007-2010 Adjunct Instructor and Research Professor, Department of Chemistry, University of Wisconsin-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

I have taught the following courses in the past six years:

Biophysical Chemistry (CHEM 406 in Fall 2015 and Fall 2016, Fall 2017, Fall 2020, Fall 2021)

Physical Chemistry 2 (CHEM 434) Spring 2017, 2018

Physical Chemistry 1 (CHEM 433) in Fall 2012, 2013 & 2014; Fall 2018

Applied Physical Chemistry (CHEM 405) Spring 2013;
General Chemistry (CHEM 109): Spring 2015, Spring 2019, Spring 2021
General Chemistry Lab: Fall and Spring 2015, Fall and Spring 2017, Fall and Spring 2018, Spring 2019,
Fall 2020

Courses with Integrating 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 Super-Computing 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

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

Major Internal Grant

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

AWARDS

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

RESEARCH WITH UNDERGRADUATE STUDENTS

We use experiment, theory, literature review, and advanced computer simulation methods to explore behaviors of molecules in complex chemical environments. I have maintained an active research program after joining the Chemistry department and was able to publish a total of 20 peer-reviewed publications with a total of **75** undergraduate students, who participated in these research studies.

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

1. *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 (2021) *ACS Bio & Med Chem Au.*, in press
2. *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, (2021) *Protein Science*, 30, 2206–2220.
<https://onlinelibrary.wiley.com/doi/10.1002/pro.4190>.
3. *Impact of Thiol-Disulfide Balance on the Binding of Covid-19 Spike Protein with Angiotensin Converting Enzyme 2 Receptor*, S. Hati and S. Bhattacharyya. (2020) *ACS Omega*, 5(26):16292-16298 <https://doi.org/10.1021/acsomega.0c02125>
4. *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. (2020) *ACS Catal.*, 10, 10229–10242.
<https://doi.org/10.1021/acscatal.0c02381>
5. *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 (2020) *Protein J.* (2020). <https://doi.org/10.1007/s10930-020-09910-3>. (Chem. 406 project).
6. *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* (2020), **Protein J.** 39(6):644-656. doi: 10.1007/s10930-020-09935-8.
7. *Crowder-Induced Conformational Ensemble Shift in Escherichia coli Prolyl-tRNA Synthetase* Adams*, L. M., Andrews*, R. J., Hu*, Q. H., Schmit*, H. L., Hati, S., Bhattacharyya, S. (2019) **Biophys. J.**, 117, 1269-1284.
 8. *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*, Hati, S., Bhattacharyya, S. (2018) **ACS Catal.** 12, 12015-12029.
 9. *Integrating Research into the Curriculum – A Low-cost Strategy for Promoting Undergraduate Research* S. Hati, , and S. Bhattacharyya, (2018) in "**Best Practices for Supporting and Expanding Undergraduate Research in Chemistry**", book chapter, American Chemical Society, Eds. Gourley, B. L. and Jones, R. M., 119-141.
 10. *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. Huntv, K. A. Jansenv, A. H. Xiong*, S. Hati, and S. Bhattacharyya (2016) **J. Mol. Model.**, 22, 199-213.
 11. *Incorporating modeling and simulations in undergraduate biophysical chemistry course to promote understanding of structure-dynamics-function relationships in proteins* S. Hati and S. Bhattacharyya (2016) **Biochem. Mol. Biol. Educ.**, 44, 140-59.
 12. *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.*, Reinhardt, C. R.*, Bartholow, T. *, Rumpel, J. P.*, North, M. A.*, and Bhattacharyya, S. (2015) **J. Phys. Chem. A**, 119, 172–182.
 13. *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 (2014) **The Protein Journal**, 33, 184-98.
 14. *Probing the global and local dynamics of aminoacyl-tRNA synthetases using all-atom and coarse-grained simulations* A. Strom*, S. Fehling*, S. Bhattacharyya, S. Hati (2014) **J. Mol. Model.**, 20, 2245-55.
 15. *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 (2014) **Biochemistry**, 53, 1059-68.
 16. *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. (2013) **Biochemistry**, 52, 4399-4412.
 17. *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. (2012) **Biochemistry**, 51, 2146-56.
 18. *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. (2011) **J. Phys. Chem. B**, 115, 3632-3641.
 19. *Improved density functional description of the electrochemistry and structure-property descriptors of substituted flavins* M. A. North*, S. Bhattacharyya, D. G. Truhlar (2010) **J. Phys. Chem. B**, 114, 14907–14915.

20. *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, (2009) **J. Phys. Chem. B**, 113, 8149-8157.
21. *Evolutionary basis for the coupled-domain motions in Thermus thermophilus leucyl-tRNA synthetase* K. Weimer*, B. Shane*, M. Brunetto, S. Bhattacharyya, and S. Hati. (2009) **J. Biol. Chem.**, 284, 10088-10099.

SERVICE AND SYNERGISTIC ACTIVITIES

- Serving as a co-lead in the writing sub-committee for the equity, diversity, and inclusion strategic planning of UW-Eau Claire
- Serving as a member of College of Arts and Sciences Curriculum Committee member
- Served as an organizer mentor for the faculty subcommittee of national computational chemistry consortium, MERCURY
- Serving as the chair for the equity, diversity, and inclusion committee of Department of Chemistry and Biochemistry
- Since 2013, I am acting as principal coordinator for Blugold Supercomputing Cluster Consortium (BSCC). Currently, I am coordinating with LTS and purchasing for installing new computing nodes
- Since Fall 2019, a part of the BGSC.ADMIN team, in order to provide assistances to the campus computing community, BSCC
- Advised research students for their post-UWEC career
- Written recommendation letters for students
- Advised chemistry major students
- Acted in departmental committees, such as general chemistry curriculum, award committee
- Served in the search committee of the director of UWEC McNair Program
- Academic Journal Manuscript Reviewer for various scientific journals. Reviewed manuscripts for 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.
- Led a collaborative effort with 17 faculty members from various departments within UW-Eau Claire to acquire funding for establishing a University-wide supercomputing cluster.
- Integrated computational quantum chemistry-based in-class authentic research projects in *Physical Chemistry (CHEM. 433)* and *Biophysical Chemistry (CHEM 406)* classroom.