

Vivek Shankar Bharadwaj

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EDUCATION

Doctor of Philosophy, Chemical Engineering Colorado School of Mines, Golden, CO	2010 – 2015
Master of Science, Chemical Engineering Colorado School of Mines, Golden, CO	2010 – 2015
Bachelor of Technology, Chemical Engineering Sardar Vallabhbhai National Institute of Technology, Surat, India	2004 – 2008

PROFESSIONAL EXPERIENCE

Sr. Staff Scientist – Computational Molecular Science National Renewable Energy Laboratory, Golden, CO	Jun 2023 – Present
<ul style="list-style-type: none">Principal Investigator (PI) on Department of Energy (Basic Energy Sciences) projects (totaling \$1.8million) on<ul style="list-style-type: none">Understanding structure and function of complex carbohydrates in plantsIntegrating computational structural biology pipelines with experiments for efficient drug-designUnderstanding the interfacial science of polymer deconstruction during hydrothermal liquefactionKey contributor in the Center for Bioenergy Innovation a DOE-BER Bioenergy Research Center. I lead the integration of experimental data with computational models to probe plant cell wall architecture and discover enzymatic mechanisms of biomass biosynthesis and deconstruction.As a Co-PI, I lead computational efforts to<ul style="list-style-type: none">Develop machine learning (ML) and artificial intelligence (AI) models for (bio)catalysisStudy charge transport in biology and energy storage materialsIntegrate molecular dynamics approaches with experimental structural biologyI also lead development of funding proposals with academia and projects with industry partners.	
Staff Scientist – Computational Molecular Science National Renewable Energy Laboratory, Golden, CO	Jun 2018 – Jul 2023
Post-Doctoral Researcher – Computational Biophysics National Renewable Energy Laboratory	Sep 2015 – May 2018
Process Engineer Hindustan Petroleum Corporation Limited	2008 – 2010

Skills & Proficiencies

- Expert at classical, enhanced sampling molecular dynamics (MD) of condensed phase (bio)molecular systems.
- Extensive experience with electronic structure calculations, hybrid quantum mechanics/molecular mechanics (QM/MM) and quantum computing for evaluating chemical/enzymatic reaction mechanisms.
- Adept at developing and utilizing ML/AI tools for foundational science in chemistry and biology.
- Proficient with methodologies for protein structure prediction, docking and binding energy calculations.
- Adept at finite element methods (FEM) to model reaction-coupled multiphysics in chemical catalytic systems.
- Proficiency with scientific computing packages: AMBER, CHARMM, Gaussian, COMSOL, AMReX, RDKit, scikit-learn.
- Programming: Python, Fortran, Linux BASH scripting, Matlab.
- Basic experience with HPLC, UV-vis and NMR spectroscopy.

PUBLICATIONS ([Google Scholar Profile](#))

(†Indicates equal contribution | *Indicates corresponding author)

- [1] Hennen, S.; Bomble, Y.; Urbanowicz, B.; **Bharadwaj, V.S.***; *Decoding substrate specificity determining factors in glycosyltransferase-B enzymes - Insights from machine learning models*, Under review in *Digital Discovery*
- [2] Wilson, W.N.; Lane, J.M.; Saha, C.; Severin, S.; **Bharadwaj, V.S.***; Rai, N.*; *Nature of molybdenum carbide surfaces for catalytic hydrogen dissociation using machine-learned potentials: an ensemble-averaged perspective*, *Catalysis Science and Technology*, (2025)
- [3] Kisgeropoulos, E.C.; **Bharadwaj, V.S.**; Ledinina, A.; Lubner C.E.; Mulder, D.W.; Smolinski, S.L.; Boehm, M.; Gutekunst, K.; King, P.W.; Drazenka, S.; *Structural and biophysical properties of a [4Fe4S] ferredoxin-like protein from Synechocystis sp. PCC 6803 with a unique two domain structure*, *Journal of Inorganic Biochemistry*, (2024)
- [4] Addison, B.A†; Bu, L.†; **Bharadwaj, V.S.†**; Crowley, M.F.; Ware, A.E.H.; Crowley, M.F.; Bomble, Y.J.; Ciesielski, P. N.; *Atomistic, macromolecular model of the Populus secondary cell wall informed by solid-state NMR*, *Science Advances*, (2024)
- [5] Zhang, L.; Prabhakar, P.K.; **Bharadwaj, V.S.**; Bomble, Y.J.; Peña, M.J.; Urbanowicz, B.R.; *Glycosyltransferase family 47 (GT47) proteins in plants and animals*, *Essays in Biochemistry*, (2023)
- [6] Prabhakar, P.K.; Pereira, J.H.; Taujale, R.; Shao, W.; **Bharadwaj, V.S.**; Chapla, D.; Yang, J-Y; Bomble, Y.J.; Moremen, K.W.; Kannan, N.; Hammel, M.; Adams, P.D.; Scheller, H.V.; Urbanowicz, B.R.; *Structural and biochemical insight into a modular β -1, 4-galactan synthase in plants*, *Nature Plants*, (2023)
- [7] Kisgeropoulos, E.C.; **Bharadwaj, V.S.**; Mulder, D.W.; King, P.W.; *The contribution of proton-donor pKa on reactivity profiles of [FeFe]-hydrogenases*, *Frontiers in Microbiology*, (2022)
- [8] Lubner C.E.; Artz J.H; Mulder, D.W.; Oza, A.; Ward, R. J.; Williams, G.; Jones, A.K.; Peters, J.W.; Smalyukh I.I.; **Bharadwaj, V.S.**; King, P.W.; *A site-differentiated [4Fe-4S] cluster controls electron transfer reactivity of Clostridium acetobutylicum [FeFe]-hydrogenase I*, *Chemical Science*, (2022)
- [9] **Bharadwaj, V.S.***; Westawker, L.P.; Crowley, M.; *Towards Elucidating Structure-Spectra Relationships in Rhamnogalacturonan II - Computational Protocols for Accurate ^{13}C and ^1H Shifts for Apiose and its Borate Esters*. *Frontiers in Molecular Biosciences*, (2022)
- [10] Wang H-T†, **Bharadwaj, V.S.†**; Yang, J.; Curry, T.M.; Moremen, K.W.; Bomble, Y.J.; Urbanowicz, B.R. *Rational enzyme design for controlled functionalization of acetylated xylan for cell-free polymer biosynthesis*, *Carbohydrate Polymers*, (2021)
- [11] Mallarapu A.†; **Bharadwaj, V.S. †***; Santhanagopalan S.*; *Understanding extreme fast charge limitations in carbonate mixtures*, *Journal of Materials Chemistry A*, (2021)
- [12] **Bharadwaj, V.S.***; Crowley, M.; Peña, M.; Urbanowicz, B.; O'Neill, M. A.; *Mechanism and Reaction Energy Landscape for Apiose Cross-Linking by Boric Acid in Rhamnogalacturonan II*. *Journal of Physical Chemistry B*, (2020)
- [13] Addison, B.; Stengel, D.; **Bharadwaj, V.S.**; Happs, R.M.; Doeppke, C.; Wang, T.; Bomble, Y.B.; Holland, G.P.; Harman-Ware, A.E.; *Selective One-Dimensional ^{13}C - ^{13}C Spin-Diffusion Solid-State Nuclear Magnetic Resonance Methods to Probe Spatial Arrangements in Biopolymers Including Plant Cell Walls, Peptides, and Spider Silk*. *Journal of Physical Chemistry B*, (2020)
- [14] O'Neill, M. A.; Black, I.; Urbanowicz, B.; **Bharadwaj, V. S.**; Crowley, M.; Koj S.; Peña, M.; *Locating Methyl-Etherified and Methyl-Esterified Uronic Acids in the Plant Cell Wall Pectic Polysaccharide Rhamnogalacturonan II*. *SLAS Technology*, (2020)

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- [15] Lunin, V.V.†; Wang H-T†, **Bharadwaj, V.S.†**; Alahuhta, M.†; Peña, M.J.; Yang, J.; Archer-hartmann, S.A., Azadi Parastoo; Himmel, M.E.; Moremen, K.W.; York, W.S.; Bomble, Y.J.; Urbanowicz, B.R. *Molecular mechanism of polysaccharide acetylation by the Arabidopsis xylan O-acetyltransferase XOAT1. The Plant Cell*, (2020)
- [16] **Bharadwaj, V. S.**; Knott, B. C.; Ståhlberg, J.; Beckham, G. T.; Crowley, M. F. *The hydrolysis mechanism of a GH45 cellulase and its potential relation to lytic transglycosylase and expansin function. Journal of Biological Chemistry*, (2020)
- [17] Ciesielski, P. N.; Pecha, M. B.; Lattanzi, A. M.; **Bharadwaj, V. S.**; Crowley, M. F.; Bu, L.; Vermaas, J. V.; Steirer, K. X.; Crowley, M. F. *Advances in multiscale modeling of lignocellulosic biomass. ACS Sustainable Chemistry and Engineering*, (2020)
- [18] Lattanzi, A. M., Pecha, M. B., **Bharadwaj, V. S.** & Ciesielski, P. N. *Beyond the effectiveness factor: Multi-step reactions with intraparticle diffusion limitations. Chemical Engineering Journal*, (2020)
- [19] **Bharadwaj, V.S**; Pecha, B.M.; Lebarbier Dagle, V.; Dagle, R.A.; Ciesielski, P.; *Multi-scale simulation of reaction, transport and deactivation in SBA-16 supported catalysts for the conversion of ethanol to butadiene. Catalysis Today* (2019)
- [20] Ciesielski, P.; Wagner R.; **Bharadwaj, V.S**; Killgore, J.; Mittal, A.; Beckham G.T.; Decker, S.R.; Himmel, M.E.; Crowley,M.F.; *Nanomechanics of cellulose deformation reveal Molecular defects that facilitate natural deconstruction. Proceedings of the National Academy of Sciences* (2019)
- [21] **Bharadwaj, V.S**; Kim, S.; Guarnieri, M.; Crowley,M.F.; *Different substrate behaviors in a P450 decarboxylase and hydroxylase reveal reactivity-enabling actors. Scientific Reports* (2018)
- [22] Ciesielski, P.; Pecha, B.M.; **Bharadwaj, V.S**; Mukarakate, C.; Leong, G.; Kappes, Branden; Crowley,M.F. ; Kim, S.; Foust, T; Nimlos,M. ; *Advancing catalytic fast pyrolysis through integrated multiscale modeling and experimentation: Challenges, progress and perspectives. WIREs: Energy and Environment* (2018)
- [23] Urbanowicz, B.R.†; **Bharadwaj, V.S.†**; Alahuhta, M.; Peña, M.J.; Lunin, V.V.; Bomble, Y.J.; Wang, S.; Yang, J.; Tuomivaara, S.T.; Himmel, M.E.; Moremen, K.W.; York, W.S.; Crowley, M.F.; *Structural, mutagenic and in silico studies of xyloglucan fucosylation in arabidopsis thaliana suggest a water-mediated mechanism. The Plant Journal* (2017) (Cover Article)
- [24] Schutt, T.; Hegde G.A.; **Bharadwaj, V.S.**; Johns A.J.; Maupin, C.M.; *Impact of water-dilution on the biomass solvation properties of the ionic liquid 1-methyltriethoxy-3-ethylimidazolium acetate. Journal of Physical Chemistry B* (2017)
- [25] Schutt, T.; **Bharadwaj, V.S.**; Hegde G.A.; Johns A.J.; Maupin, C.M.; *In silico insights into the solvation characteristics of the ionic liquid 1-methyltriethoxy-3-ethylimidazolium acetate for cellulosic biomass. Physical Chemistry Chemical Physics* (2016)
- [26] Hegde G.A.; **Bharadwaj, V.S.**; Kinsinger C.L.; Schutt, T.; Pisierra N.R.; Maupin, C.M.; *Impact of water dilution and cation tail length on ionic liquid characteristics: Interplay between polar and non-polar interactions. The Journal of Chemical Physics* (2016)
- [27] **Bharadwaj, V. S.**; Eagan, N.; Wang, N.; Liberatore, M.W.; Maupin, C.M.; *Molecular simulations of fatty acid methyl esters and representative biodiesel mixtures. ChemPhysChem* (2015) (Cover Article)
- [28] Schutt, T. †; **Bharadwaj, V. S.†**; Maupin, C.M.; *The impact active site protonation on substrate ring conformation in Melanocarpus albomyces Cellobiohydrolase Cel7B. Physical Chemistry Chemical Physics* (2015)
- [29] **Bharadwaj, V. S.**; Schutt, T.; Ashurst, T.; Maupin, C.M.; *Elucidating the conformational energetics of glucose and cellobiose in ionic liquids. Physical Chemistry Chemical Physics* (2015)

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- [30] **Bharadwaj, V. S.**; Vyas, S.; Villano, S. M.; Maupin, C.M; and Dean, A. M.; *Unravelling the impact of hydrocarbon structure on the fumarate addition mechanism – a gas-phase ab-initio study. Physical Chemistry Chemical Physics* (2015) **(Featured on the Issue Back Cover)**
- [31] Sambasivarao, S. V.; Roberts, J.; **Bharadwaj, V. S.**; Slingsby, J. G.; Rohleder, C.; Mallory, C.; Groome, J. R.; McDougal, O. M.; Maupin, C. M, *Acetylcholine promotes binding of α -conotoxin MII for $\alpha 3\beta 2$ nicotinic acetylcholine receptors. ChemBioChem* (2014) **(Cover Article)**
- [32] **Bharadwaj, V. S.**; Dean, A. M.; and Maupin, C.M., *Insights into the glycy radical enzyme active site of benzy succinate synthase: A computational study. Journal of the American Chemical Society* (2013)
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CONFERENCE PRESENTATIONS & INVITED TALKS

- **Bharadwaj, V. S.**, Computational investigations of complex carbohydrate systems: Sequence-structure-function relationships and beyond. (Feb 2025) *Complex Carbohydrate Research Center, University of Georgia, Athens, USA (Invited)*
- **Bharadwaj, V. S.**, In-silico investigations of bio-inorganic constructs: from plant cell walls to electron transport. (May 2023) *8th Georgian Bay International Conference on Bioinorganic Chemistry in Parry Sound, Canada. (Invited)*
- **Bharadwaj, V. S.**, *The Curious Cases of Water as a Shuttle, Scissors and a Barricade* - Unlocking Enzymatic Mechanisms Across the Biomass Life Cycle with Molecular Simulations. (Feb 2021) *Department of Chemistry, Virtual Seminar, Colorado School of Mines. (Invited)*
- **Bharadwaj, V. S.**, Unravelling Catalytic Mechanisms Across the Biomass Life Cycle Using Molecular Simulations. (Sept 2020) *Chemical Engg. Department Virtual Seminar, Mississippi State University. (Invited)*
- **Bharadwaj, V. S.**, From Molecular Modeling to Multiscale - Computational Approaches to Advancing Bioenergy Science and Technology (Sept 2019) *US Army ERDC Jackson, MS. (Invited)*
- **Bharadwaj, V. S.**, Advancing Bioenergy Science with Computational Lenses: Elucidating Enzymatic Mechanisms with Molecular Modelling. (Jan 2019) *Department of Biotechnology Indian Institute of Technology Madras, Chennai, TN, India. (Invited)*
- **Bharadwaj, V. S.**, Extracting Transport Independent Kinetics for Vapor Phase Upgrading of Biomass Pyrolysis Vapors over H-ZSM-5. (Oct 2018) *AIChE Annual Meeting, Pittsburg, PA.*
- **Bharadwaj, V. S.**, Addressing Issues in a Bioenergy Economy with Molecular Modelling Approaches. (Feb 2018) *Intel Corporation, Hillsboro, OR. (Invited)*
- **Bharadwaj, V. S.**, Xyloglucan Fucosylation in *Arabidopsis thaliana* – A Water Mediated Mechanism. (Fall 2017) *254th ACS National Meeting, Washington DC.*
- **Bharadwaj, V. S.**, Hydrolysis Mechanisms in GH45: A Segue to Understanding Expansin Action. (Fall 2017) *Gordon Research Seminar on Cellulases & other Carbohydrate-Active Enzymes, Andover NH. (Invited)*
- **Bharadwaj, V. S.**, Enabling Alternative Fuel Applications Through Fundamental Computational Studies. (Fall 2015) *National Renewable Energy Laboratory, Golden CO. (Invited)*
- **Bharadwaj, V. S.**, Schutt, T., Ashurst, T. and Maupin, C.M. How Ionic Liquids Effect Glucose and Cellobiose Solvation; Insights from Enhanced Sampling Molecular Dynamics Techniques (Spring 2015) *249th ACS National Meeting, Denver, CO.*
- **Bharadwaj, V. S.**, Dean, A. M., and Maupin, C.M. Impact of Hydrocarbon Fuel Structure on Anaerobic Biodegradation via the Fumarate Addition Reaction: An Ab-Initio and Kinetic Modelling Study. (Nov 2014) *The AIChE Annual meeting, Atlanta GA.*
- **Bharadwaj, V. S.**, Dean, A. M., and Maupin, C.M. Computational Insights into Enzymatic Free Radical Chemistry and its Role in the Bio-degradation of Toluene: The Case of Benzy succinate Synthase from Structure to Mechanisms (Nov 2014) *The AIChE Annual meeting, Atlanta GA.*
- **Bharadwaj, V. S.**, Schutt, T., Ashurst, T. and Maupin, C.M. Impact of Ionic Liquids on Cellulose (Summer 2014) *AAAS Pacific Division Annual Meeting, UC Riverside.*

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- **Bharadwaj, V. S.,** Dean, A. M., and Maupin, C.M. Computational structural elucidation of benzylsuccinate synthase: A bridge to understanding free-radical chemistry in the anaerobic biodegradation of hydrocarbons, (Fall 2012) 244th ACS National Meeting, Philadelphia PA.
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AWARDS

- NREL President's Award for exceptional performance (2024)
 - Key-contributor award recognizing exceptional performance in the BioEnergy Science and Technology Directorate at NREL for FYs-2018, 2020, 2021, 2022, 2023, 2024.
 - Outstanding mentor award for DOE's science undergraduate and graduate internship programs (2020, 2024)
 - Chemical Computing Group (CCG) Research Excellence award at the 249th ACS National Meeting Denver (Spring 2015)
 - NVIDIA Best GPU Poster Award at the 248th ACS National Meeting San Francisco (Fall 2014)
 - NSF Travel Grant to attend the PASI (Pan-American Advanced Studies Institute) workshop on Molecular-based Multiscale Modeling and Simulation, Montevideo, Uruguay (Sept 2012)
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TEACHING AND MENTORING

- Mentored 5 students under DOE's Science Undergraduate Learning Internship (SULI) program Summer 2020-Present.
 - Teaching Assistant (Fall 2014 & Fall 2015): CBEN 698/498 – Molecular-level Computations and Simulations – Prof. C. Mark Maupin.
 - Co-developed course work and lab assignments.
 - Teaching Assistant (Fall 2010): DCGN210A - Introduction to Thermodynamics – Prof. Charles Vestal.
 - Mentored undergraduates on the principles and applications of molecular simulation techniques under the Research Experience for Undergraduates (REU) program.
 - Taught high-school students the fundamentals of computational chemistry and their applications in research as part of the group's outreach activities (Summer 2013 & Summer 2014).
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PROFESSIONAL SERVICES

- Associate editor for the journal Frontiers in Plant Science.
 - Session Co-Chair for the session titled "Machine Learning for Soft and Hard Materials" AICHE 2025.
 - Peer-review referee for JPCB, JCIM (ACS publications); RSC Advances, Catalysis Science and Technology (Royal Society of Chemistry); Carbohydrate Research (Elsevier publications); Catalysts, Molecules, Polymers, IJMS (MDPI publications).
 - Member of the American Chemical Society & American Institute of Chemical Engineers.
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LEADERSHIP

- Department (ChBE) Representative in the Graduate Student Government at CSM (2014-2015)
 - President (2012-2014) and Web-Secretary (2011) of Indian Student Association at CSM
 - Student Council Representative SVNIT Surat for the year 2005-06 (2nd year B-Tech Chemical Engg.)
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REFERENCES

Shall be provided upon request.
