

Dalia R. Biswas, Ph.D.

Associate Professor, Department of Chemistry, Whitman College

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Education and Academic Positions

Associate Professor, Department of Chemistry, Whitman College (2017-present)
Assistant Professor, Department of Chemistry, Whitman College (2011-17)
Visiting Assistant Professor, Department of Chemistry, Whitman College (2010-11)
Postdoctoral Research Associate, Montana State University, Bozeman, MT (2005-10)
Ph.D. in Inorganic Chemistry, The University of Montana, Missoula, MT (2000-05)
B. Sc. (Honors) in Chemistry, Jahangirnagar University, Dhaka, Bangladesh (1994-98)

Honors and Awards

Suzanne L. Martin Award for Excellence in Mentoring, Whitman College, 2017-18
Outstanding Foreign Student Award, The University of Montana, 2005
Diversity Student Achievement Award, The University of Montana, 2005
Bertha Morton Scholarship for outstanding graduate student, The University of Montana, 2002
Lola Walsh Anacker Scholarship for outstanding female graduate student, Department of Chemistry, The University of Montana, 2002

Teaching Experience

Whitman College, Walla Walla, Washington (2010-present)

- General Chemistry (CHEM-125/126)
- Advanced General Chemistry (CHEM-140)
- Organic Chemistry Laboratory I and II (CHEM-251/252)
- Computational Chemistry (CHEM-275)
- Inorganic Chemistry (CHEM-360)
- Advanced Synthesis (CHEM-370)
- Biochemistry (BBMB-325)
- Computational Biochemistry (CHEM-425)

Montana State University, Bozeman, Montana (2007-2010)

- Supervised REU and undergraduate students in protein expression, purification, and characterization using various spectroscopic techniques (2007-2010)
- Introduction to Organic and Biochemistry (CHMY-123, Spring 2010)
- Principles of Biochemistry (BCHM-340, Summer 2009)

Teaching Assistant at The University of Montana, Missoula, MT (2000-2005)

- General and Inorganic Chemistry
- Organic and Biochemistry
- Organic Chemistry (200 level)
- Inorganic Chemistry Lab (400 level)

Research Experience

Max Planck Institute for Chemical Energy Conversion, Germany (Feb-May 2014)

- Developed and implemented QM/MM models on CODH enzyme
- Collaborated with Dr. Marius Retegan and Prof. Frank Neese

Montana State University, Bozeman, MT (2005-2010)

- Conducted active site modeling of Cu-proteins using quantum mechanics (QM) methods
- Experienced in protein expression, purification, and characterization using various spectroscopic techniques (XAS, UV/VIS, CD/MCD, EPR)

The University of Montana, Missoula, MT (2000-2005)

- Experienced in organometallic synthesis, working with inert atmosphere glove boxes, cyclic voltammetry, and various spectroscopic techniques (NMR, UV/VIS, FTIR)

- Investigated the electronic structure of organometallic systems using DFT calculations

Professional Association

- American Chemical Society (ACS) (2000 – present)
- Society of Biological Inorganic Chemistry (SBIC)
- American Association of University Professor (AAUP)
- NSF Center for Computer Assisted Synthesis (2023 – Present)

Reviewer

- Analytical biochemistry
- ASME International Mechanical Engineering Congress and Exposition
- Journal of Cluster Science
- Protein Science
- National Science Foundation Grants
- Murdock Charitable Trusts

Committee Served (Whitman College)

- Curriculum Committee (2017-2020)
 - Chair of Curriculum Committee 2019-20
- Student Life Committee (Jan-May, 2012)
- Office of Off-campus Studies (2011-2013)
- Scholars at Risk (2018-19)
- Campus Affairs – Library committee (2024-present)

Funded Research

External Grants

4. NSF Center for Computer-Assisted Synthesis, “Heteroaromatic Aryne Chemistry: Data Science, Computational, and Synthetic Studies” (\$56,489, **2024-25**), Co-PIs (in alphabetical order): D. Biswas (Whitman), J. Kisunzu (Colorado College), R. Paton (Colorado State).
3. National Science Foundation “RUI: Study of Small Molecule Activation by Molybdenum Enzymes using QM and QM/MM Methods” (\$188,386, **2018-2021**), PI
2. National Science Foundation, "RUI: The Sources of Substrate Specificity in Enzymes Hydroquinone Dioxygenases", (\$385,400, **2015-2018**), Co-PIs: Tim Machonkin, Doug Juers, and Dalia Rokhsana.
1. Murdock College Research Program for Natural Sciences (\$59,600 plus \$14,400 matching funds from Whitman College, **2015-17**) "Realistic computational and synthetic models for structure/function studies of Mo-Cu containing carbon monoxide dehydrogenase" PI

Whitman College Internal Grants

9. Robert Norton Summer Research Award with Lindsay Farr (\$5,540, **2019**), "Developing Computational Models for Molybdenum-Enzyme"
8. Louis B. Perry Student-Faculty Research Award with Laurinda Nyarko (\$7,500, **2018**), "Inorganic Model Complexes Potential for Hydrogen Gas Production"

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7. Louis B. Perry Student-Faculty Research Award with Laurinda Nyarko (\$3,500, **2017**). "Study of Bioinspired Metal Complexes using Computational and Synthetic Approaches"
6. Louis B. Perry Student-Faculty Research Award with Morgan Dienst and Jacob O'Conner (\$8,500, **2014**) "QM/MM Investigation of Mo-Containing Carbon Monoxide Dehydrogenase"
5. Whitman Internship Grant for Peter Carmichael (\$2,500, **2014**) "Investigation of a Bacterial Enzyme (PcpA) using QM and QM/MM Methods"
4. Louis B. Perry Student-Faculty Summer Research Award with Morgan Dienst and Daniel Ellis (\$8,500, **2013**) "Computational Modeling and Biomimetic Synthesis of the Active Site of Carbon Monoxide Dehydrogenase"
3. Robert Norton Science Summer Research Award for Tao Large (\$3,000, **2013**) "Computational Modeling and Biomimetic Synthesis of the Active Site of Carbon Monoxide Dehydrogenase"
2. Louis B. Perry Student-Faculty Research Award with Morgan Dienst (\$8,500, **2012**) "Computational Modeling and Biomimetic Synthesis of the Active Site of Carbon Monoxide Dehydrogenase"
1. HHMI Student-Faculty Research Award with Daniel Ellis and Gus Friedman (\$5,000, **2012**), "Computational Modeling and Biomimetic Synthesis of the Active Site of Carbon Monoxide Dehydrogenase"

Publications

19. Lim, H.; Baker, M.L.; Cowley, R.E.; Kim, S.; Bhadra, M.; Siegler, M.A.; Kroll, T.; Sokaras, D.; Weng, T-C.; Biswas, D.R.; Dooley, D.M.; Karlin, K.D.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. "K β X-ray Emission Spectroscopy as a Probe of Cu(I) Sites: Application to the Cu(I) Site in Preprocessed Galactose Oxidase." *Inorganic Chemistry*, **2020**, 59(22), 16567-16581 (DOI: 10.1021/acs.inorgchem.0c02495)
18. Cowley, R.E.; Cirera, J.; Qayyum, M. F.; Rokhsana, D.; Hedman, B.; Hodgson, K. O.; Dooley, D.M.; Solomon, E. I. Structure of the Reduced Copper Active Site in Pre-Processed Galactose Oxidase: Ligand Tuning for One-Electron O₂ Activation in Cofactor Biogenesis, *Journal of American Chemical Society*, **2016**, 138 (40), 13219-13229 (DOI: 10.1021/jacs.6b05792)
17. Rokhsana, D.; Large, T.; Dienst, M.; Retegan, M., Neese, F. A realistic in silico model for structure/function studies of molybdenum-copper CO dehydrogenase, *Journal of Biological Inorganic Chemistry*, **2016**, 21, 491-499 (DOI: 10.1007/s00775-016-1359-6)
16. Schofield, J. A.; Brennessel, W. W.; Urnezius, E.; Rokhsana, D.; Boshart, M. D.; Juers, D. H.; Holland, P. L. and Machonkin, T. E. (2015), Metal-Halogen Secondary Bonding in a 2,5-Dichlorohydroquinonate Cobalt(II) Complex: Insight into Substrate Coordination in the Chlorohydroquinone Dioxygenase PcpA. *European Journal of Inorganic Chemistry*, **2015**: 4643-4647 (DOI: 10.1002/ejic.201500845)
15. Machonkin, T. E.; Boshart, M. D.; Schofield, J. A.; Rodriguez, M. M.; Grubel, K.; Rokhsana, D.; Brennessel, W. W.; Holland, P. L. Structural and Spectroscopic Characterization of Iron(II), Cobalt(II), and Nickel(II) Ortho-Dihalophenolate Complexes: Insights into Metal-Halogen Secondary

Bonding, *Inorganic Chemistry*, **2014**, 53(18), 9837-9848 (DOI: 10.1021/ic501424e)

14. Rokhsana, D.; Howells, A. E.; Dooley, D. M.; Szilagyi, R. K. "The Role of the Tyr-Cys Crosslink to the active site properties of galactose oxidase" *Inorganic Chemistry*, **2012**, 51(6), 3513-3512. (DOI: 10.1021/ic2022769)

13. Rokhsana, D.; Shepard, E. M.; Brown, D. E.; and Dooley, D. M. (2011) Amine Oxidase and Galactose Oxidase, in Copper-Oxygen Chemistry (eds K. D. Karlin and S. Itoh), John Wiley & Sons, Inc., Hoboken, NJ, USA. (DOI: 10.1002/9781118094365.ch3)

12. Begum, N.; Hyder, M. L.; Hassan, M. R.; Kabir, S. E.; Bennett, D. W.; Haworth, D. T.; Siddiquee, T. A.; Rokhsana, D.; Sharmin A.; Rosenberg, E. "Facile E-E and E-C bond activation of PhEPh (E = Te, Se, S) by ruthenium carbonyl clusters: Formation of Di- and triruthenium complexes bearing bridging dppm and phenylchalcogenide and capping chalcogenido ligands" *Organometallics*, **2008**, 27, 1550-1560 (DOI: 10.1021/om701042s)

11. Rokhsana, D.; Dooley, D. M.; Szilagyi, R. K. "Systematic development of computational models for the catalytic site in galactose oxidase: impact of outer-sphere residues on the geometric and electronic structures" *Journal of Biological Inorganic Chemistry*, **2008**, 13, 371-383 (DOI: 10.1007/s00775-007-0325-8)

10. Rokhsana, D.; Dooley, D. M.; Szilagyi, R. K. "Structure of the oxidized active site of galactose oxidase from realistic *in silico* models" *Journal of the American Chemical Society*, **2006**, 128(49), 15550-15551 (DOI: 10.1021/ja062702f)

9. Begum, N.; Hyder, Md. I.; Kabir, S. E.; Hossain, G. M. G.; Nordlander, E.; Rokhsana, D.; Rosenberg, E. "Dithiolate complexes of manganese and rhenium: X-ray structure and properties of an unusual mixed valence cluster $Mn_3(CO)_6(\mu-\eta^2-SCH_2CH_2CH_2S)_3$ " *Inorganic Chemistry*, **2005**, 44(26), 9887-9894 (DOI: 10.1021/ic050987b)

8. Mottalib, Md. A.; Begum, N.; Abedin, S. M. T.; Akter, T.; Kabir, S. E.; Miah, Md. A.; Rokhsana, D.; Rosenberg, E.; Hossain, G. M. G.; Hardcastle, K. I. "Reactions of electron-deficient triosmium clusters with diazomethane: electrochemical properties and computational studies of charge distribution" *Organometallics*, **2005**, 24(20), 4747-4759 (DOI: 10.1021/om0503794)

7. Kabir, S. E.; Miah, Md. A.; Sarker, N. C.; Hossain, G. M. G.; Hardcastle, K. I.; Rokhsana, D.; Rosenberg, E. "Reactions of the unsaturated triosmium cluster $[(\mu-H)Os_3(CO)_8(Ph_2PCH_2P(Ph)C_6H_4)]$ with HX (X = Cl, Br, F, CF_3CO_2 , CH_3CO_2): X ray structures of $[(\mu-H)Os_3(CO)_7(\eta^1-Cl)(\mu-Cl)_2(\mu-dppm)]$, $[(\mu-H)_2Os_3(CO)_8(Ph_2PCH_2P(Ph)C_6H_4)]^+[CF_3O]^-$ and the two isomers of $[(\mu-H)Os_3(CO)_8(\mu-Cl)(\mu-dppm)]$ " *Journal of Organometallic Chemistry*, **2005**, 690, 3044-3053 (DOI: 10.1016/j.jorganchem.2005.03.041)

6. Begum, N.; Deeming, A.; Islam, M.; Kabir, S.; Rokhsana, D.; Rosenberg, E. "Reactions of benzothiazolide triosmium clusters with tetramethylthiourea" *Journal of Organometallic Chemistry*, **2004**, 689(16), 2633-2640 (DOI: 10.1016/j.jorganchem.2004.05.023)

5. Nervi, C.; Gobetto, R.; Milone L.; Viale, A.; Rosenberg, E.; Spada, F.; Rokhsana, D.; Fiedler, J. "Solution properties, electrochemical behavior and protein interactions of water soluble triosmium carbonyl clusters" *Journal of Organometallic Chemistry*, **2004**, 689(10), 1796-1805 (DOI: 10.1016/j.jorganchem.2004.02.036)

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4. Rosenberg, E.; Rokhsana, D.; Nervi, C.; Gobetto, R.; Milone, L.; Viale, A.; Fiedler, J.; Botavina, M. A. "Synthesis, reduction chemistry, and spectroscopic and computational studies of isomeric quinoline carboxaldehyde triosmium clusters" *Organometallics*, **2004**, 23(2), 215-223 (DOI: 10.1021/om030564m)
3. Nervi, C.; Gobetto, R.; Milone, L.; Viale, A.; Rosenberg, E.; Rokhsana, D.; Fiedler, J. "Spectroscopic and computational investigations of stable radical anions of triosmium benzoheterocycle clusters" *Chemistry-A European Journal*, 2003, 9(23), 5749-5756 (DOI: 10.1002/chem.200305198)
2. Rosenberg, E.; Abedin, M. J.; Rokhsana, D.; Viale, A.; Dastru', W.; Gobetto, R.; Milone, L.; Hardcastle, K. "Ligand dependent structural changes in the acid-base chemistry of electron deficient benzoheterocycle triosmium clusters" *Inorganic Chimica Acta*, **2002**, 334, 343-354 (DOI: 10.1016/S0020-1693(02)00794-6)
1. Rosenberg, E.; Abedin, M. J.; Rokhsana, D.; Osella, D.; Milone, L.; Nervi, C.; Fiedler, J. "The electrochemical behavior of electron deficient benzoheterocycle triosmium clusters" *Inorganic Chimica Acta*, **2000**, 300-302, 769-777 (DOI: 10.1016/S0020-1693(00)00020-7)

Invited Presentations

5. Biswas, D. Structural/Mechanistic Insights of Molybdenum Enzymes from Computational Studies, Ursinus College, Collegeville, PA (April **2022**)
4. Rokhsana, D. Computational Studies of CO Dehydrogenase: Insights from QM and QM/MM simulations, Gonzaga University, Spokane, WA (April, **2016**).
3. Rokhsana, D.; Large, T.; Dienst, M.; Retegan, M.; Neese, F. Carbon Monoxide dehydrogenase with a unique Mo-Cu center: Structural insights from QM and QM/MM models, 69th Northwest Regional American Chemical Society Meeting, Missoula, Montana (June **2014**).
2. Rokhsana, D. Computational approach for evaluating the active site structure of metalloenzymes: Key consideration in modeling, Jahangirnagar University, Dhaka, Bangladesh (3 August, **2011**).
1. Rokhsana, D. "In silico modeling of the active site structures of Cu-proteins: What are the key elements?" organized by the Center for Biomolecular Structure and Dynamics, The University of Montana, Missoula, MT (October **2009**).

Conference Presentations

16. Biswas, D.; Study of molybdenum-containing carbon monoxide dehydrogenase using QM and QM/MM methods, (oral) ACS National Meeting, August **2023**, San Francisco, CA.
15. Biswas, D.R.; Brown, M.; Twomey, L.; Retegan, M.; Neese, F. Activation of CO by carbon monoxide dehydrogenase using QM methods (poster), International Conference on Biological Inorganic Chemistry (ICBIC-19), August 11-16, **2019**, Interlaken, Switzerland.
14. Rokhsana, D. CO Dehydrogenase: Structure-function studies from computational Simulation, Volcano Conference, March 3, **2017**, Pack Forest, WA.
13. Rokhsana, D.; Large, T.; Dienst, M.; Retegan, M.; Neese, F. Study of water splitting at the Mo-Cu

center of carbon monoxide dehydrogenase using realistic *in silico* models (oral), International Chemical Congress of the Pacific Basin Societies (PacifiChem), December 15-20, **2015**, Honolulu, HI.

12. Rokhsana, D.; Large, T.; Dienst, M.; Retegan, M.; Neese, F. Study of molybdenum-containing carbon monoxide dehydrogenase using QM and QM/MM methods, (oral) American Chemical Society National Meeting, August **2014**, San Francisco, CA.

11. Rokhsana, D.; Large, T.; Dienst, M. Computational Understanding of the active site of Molybdenum containing Carbon Monoxide Dehydrogenase (poster) International Conference on Biological Inorganic Chemistry, July **2013**, Grenoble, France.

10. Rokhsana, D.; Dooley, D. M.; Szilagyi, R. K. "Spectroscopic and theoretical investigations of the role of Tyr-Cys crosslink in galactose oxidase" (Poster) Symposium on Advance Biological Inorganic Chemistry, November **2009**, Mumbai, India.

9. Rokhsana, D.; Dooley, D. M.; Szilagyi, R. K. "Impact of the Tyr-Cys crosslink and the outer-sphere residues on the structures for the catalytic site in galactose oxidase" (poster), American Chemical Society National Meeting, March **2009**, Salt Lake City, UT.

8. Rokhsana, D.; Dooley, D. M.; Szilagyi, R. K. Impact of the Tyr-Cys crosslink and the outer-sphere residues on the structures for the catalytic site in galactose oxidase (poster), Metals in Biology, January **2009**, Ventura, CA.

7. Rokhsana, D.; Dooley, D. M.; Szilagyi, R. K. Systematic development of computational models for the catalytic site in galactose oxidase: impact of outer-sphere residues on the geometric and electronic structures (poster), International Symposium of Bio-Organometallic Chemistry, July **2008**, Missoula, MT.

6. Rokhsana, D.; Dooley, D. M.; Szilagyi, R. K. Structure of the oxidized active site of galactose oxidase from realistic *in silico* models (Oral), ACS Montana Section meeting, April **2007**, Butte, MT.

5. Rokhsana, D.; Rosenberg, E. Spectroscopic investigation of the chemically reduced 4-quinoline carboxaldehyde triosmium clusters, 58th ACS Northwest Regional Meeting, June **2003**, Bozeman, MT

4. Rokhsana, D.; Rosenberg, E.; Nervi, C.; Hardcastle, K. I. Spectroscopic studies of triosmium benzoheterocycle radical anions (oral) 57th ACS Northwest Regional Meeting, June **2002**, Spokane, WA.

3. Rokhsana, D.; Rosenberg, E.; Nervi, C.; Hardcastle, K. I. Spectroscopic studies of triosmium benzoheterocycle radical anions (oral) ACS Montana Section meeting, April **2002**, Butte, MT.

2. Rokhsana, D.; Rosenberg, E. Heterocyclic ligand cleavage of electron deficient benzoheterocycle triosmium clusters (poster) 56th ACS Northwest Regional Meeting, June **2001**, Seattle, WA

1. Rokhsana, D.; Rosenberg, E. Heterocyclic ligand cleavage of electron deficient benzoheterocycle triosmium clusters (oral), ACS Montana Section meeting, April **2001**, Butte, MT

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Service to the College and Community

- Participated as a Science Fair Judge at Whitman College for middle school students, April 2012.
- Conducted a two-hour workshop on “3D Visualization of Molecules” for 7th and 8th graders from Walla Walla public schools, organized by the Whitman Institute for Summer Enrichment (WISE) program, August 2012.
- Participated as a Science Fair Judge at the Whitman Science Fair for middle school students, March 2013.
- Organized hands-on science activities at Green Park Elementary School, Walla Walla, March 2013.
- Ran two one-hour computational workshops for 8th graders from Pioneer Middle School, organized by Mary Burt, June 2013.
- Engaged in discussion sessions with:
 - 15 students of color at Glover Alston Center, Fall 2014.
 - First-Generation Working-Class students interested in the Sciences, Fall 2014.
 - International students about classroom culture during first-year orientation, August 2015.
- Served as a faculty panelist with four minority students in the Science and Race Panel at the Power and Privilege Symposium, Spring 2015.
- Member of various search committees:
 - Three Chemistry tenure-track positions (2011, 2014, 2017).
 - Six Chemistry visiting faculty positions (2011-2021).
 - Assistant Director for Intercultural Center (Spring 2015).
 - International Student Adviser (Spring 2015).
 - Vice President of Student Affairs and Dean of Students (2016-2017).
 - Computational Chemistry Lab Technician (2021).
- Served as Search Chair for the Physical Chemistry tenure-track position (2017).
- Participated in discussions about classroom culture at International Student Orientation Camp, August 2015.
- Presided over a bioinorganic session with Prof. Denyce Wicht (Suffolk University) at the ACS National Meeting, Boston, MA, August 18, 2015.
- Participated in the Faculty Technology Showcase at Whitman College with the presentation titled “High Performance Computing,” November 2, 2015.
- Led the design and implementation of the Computational Chemistry Lab, 2019-2021.
- Served as an academic adviser for the Muslim Student Association, 2011-2019.
- Serving as an academic adviser for the South Asian Student Association, 2018-present.
- Actively advise minority students (First Generation Working Class, students of color, or international students).