Christopher N. Rowley

Department of Chemistry, Carleton University, www.rowleygroup.net

Professional Experience

Associate Professor
Department of Chemistry
Carleton University, Ottawa, ON, Canada
2021 – present

Associate Professor
Department of Chemistry
Memorial University of Newfoundland, St. John's, NL, Canada
2017 – 2020

Assistant Professor
Department of Chemistry
Memorial University of Newfoundland, St. John's, NL, Canada
2012 – 2017

NSERC Postdoctoral Fellow
Department of Biochemistry and Molecular Biology with Professor Benoît Roux
University of Chicago, Chicago, IL
2010 – 2012

Education

University of Ottawa, Ottawa, ON, Canada
Ph.D., Chemistry, 2010

Carleton University, Ottawa, ON, Canada
B.Sc. (Hons), Computational Chemistry, 2004

Research Interests

biophysical chemistry, covalent modification of proteins, molecular simulation, neural network potentials, membrane permeation, computational chemistry

Selected Awards and Honours

1. 2022 – Canadian Society for Chemistry Tom Ziegler Award
2. 2018 - Molecular Graphics and Modelling Society Frank Blaney Award
3. 2017 - American Chemical Society OpenEye Young Faculty Award

4. 2016 - President's Award for Academic Research (Memorial University)
5. 2010–2012 - NSERC Postdoctoral Fellowship
6. 2009 - University of Ottawa Faculty of Science Teaching Assistant of the Year Award
7. 2006 - Sun Microsystems of Canada Scholarship in the Computational Sciences and Engineering (2 year, $5000 pa.)
8. 2006 - NSERC Postgraduate Scholarship (Doctoral)
9. 2005 - NSERC Postgraduate Scholarship (Master's)
10. 2004 - Senate Medal for Academic Achievement (Carleton University)
11. 2003 - The Canadian Society for Chemistry Medal (Carleton University)

Publication Highlights

High Impact Publications

- **Lahey S.-L. J.**, **Rowley, C. N.**, Simulating Protein–Ligand Binding with Neural Network Potentials *Chem. Sci.*, **2020**, doi: 10.1039/C9SC06017K
- **Riahi, S.**, **Rowley C.N.** Why Can Hydrogen Sulfide Permeate Cell Membranes? *J. Am. Chem. Soc.* **2014**, 136 (43), 15111–15113, doi: 10.1021/ja508063s (59 citations)

Review Articles

- Sandeep Inakollu, V. S., Geerke, D. P., **Rowley, C. N.**, Yu, H., Polarisable force fields: What do they add in biomolecular simulations? *Curr. Opin. Struct. Biol.*, doi: 10.1016/j.sbi.2019.12.012, invited review
- **Awoonor-Williams, E., Walsh, A. G., Rowley, C. N**. Modeling Covalent-Modifier Drugs, *BBA – Proteins and Proteom.*, **2017**, doi: 10.1016/j.bbapap.2017.05.009 (27 citations)
- **Awoonor-Williams, E., Rowley C.N.** Molecular Simulation of Non-facilitated Membrane Permeation, *Biochim. Biophys. Acta - Biomembranes* **2016**, 1672–1687, doi: 10.1016/j.bbamem.2015.12.014 (59 citations)

Collaborative Research

- Vant, J., **Lahey, S-L. J.**, Jana, K., Shekhar, M., Sarkar, D., Munk, B. H., Kleinekathöfer, U., Mittal, S., **Rowley, C. N.**, Singharoy, A. Flexible fitting of small-molecules into electron microscopy maps using molecular dynamics simulations with Neural Network Potentials, *J. Chem. Inf. Model.*, special issue on Frontiers in CryoEM Modeling, DOI: 10.1021/acs.jcim.9b01167
- **Awoonor-Williams, E**; Isley III, W; Dale, S; Roux, B; Becke, A; Yu, H; Johnson, E. R.; Rowley, C. N. Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols, *J. Comput. Chem.*, **2019**, doi: 10.1002/jcc.26064
- Richmond, E., Yi, J., Vuković, V. D., **Sajadi, F.**, **Rowley, C. N.**, Moran, J., Ring-opening hydroarylation of monosubstituted cyclopropanes enabled by hexafluoroisopropanol. *Chem. Sci.* **2018**, doi: 10.1039/C8SC02126K

- Chatelain, P., Sau, A., **Rowley, C. N.**, Moran, J. The Suzuki–Miyaura Coupling of Arylsulfones, *Angew. Chem. Int. Ed.*, **2019**, doi: 10.1002/anie.201908336
- Lee, C., Comer, J., Herndon, C., Leung, N; Pavlova, A., Swift, R., Tung, **Rowley, C.N.**, Amaro, R; Chipot, C., Wang, Y., Gumbart, J. Simulation-based approaches for determining membrane permeability of small compounds *J. Chem. Inf. Model.* **2016** doi: 10.1021/acs.jcim.6b00022 (90 citations)

Full Publication List

Independent Publications

1. Isbrandt, E; Chapple, D; Tu, NTP Dimakos, V.; Beardall, AM; Boyle, P; Rowley, CN; Blacquiere , J; Newman, S. Controlling Reactivity and Selectivity in the Mizoroki–Heck Reaction: High Throughput Evaluation of 1,5-Diaza-3,7-diphosphacyclooctane Ligands *J. Am. Chem. Soc.* **2024** DOI: 10.1021/jacs.3c14612
2. Tu, NTP; Rezajooei, N.; Johnson E.R.; . Rowley, CN; A neural network potential with rigorous treatment of long-range dispersion, *Digital Discovery,* **2023**, DOI: 10.1039/D2DD00150K
3. Watt SKI; Charlebois, JG; Rowley CN; Keillor JW, A mechanistic study of thiol addition to N-acryloylpiperidine, *Org. Biomol. Chem.*, **2023**, 21, 2204-2212
4. **Montero, S.**; Booth, V.; **Rowley, C.N.** Interaction Between Antimicrobial Peptide Magainin 2 and Non-lipid Components in the Bacterial Outer Envelope, *J. Phys. Chem. B* **2022** 126 (29), 5473–5480 doi: 10.1021/acs.jpcb.2c02768
5. Abdelfatah, N.; Mostafa, A.A.; French C.R.; Doucette, L.P.; Penney, C.; Lucas, M.B.; Griffin, A.; Booth, V.; **Rowley, C.N.**; **Besaw, J.E.**; Tranebjærg, L.; Rendtorff N.D.; Hodgkinson, K.A.; Little L.A; Agrawal, S.; Parnes, L.; Batten, T.; Moore, S.; Hu, P.; Pater, J.A.; Houston, J.; Galutira, D.; Benteau, T.; MacDonald, C.; French, D.; O'Rielly, D.D.; Stanton S.G.; Young, T.-L. A Pathogenic Deletion in Forkhead Box L1 (FOXL1) Identifies the First Otosclerosis (OTSC) Gene *Human Genetics* **2022** doi: 10.1007/s00439-021-02381-1
6. **Awoonor-Williams, E**; Rowley, C.N. Modeling the Binding and Conformational Energetics of a Targeted Covalent Inhibitor to Bruton's Tyrosine Kinase *J. Chem. Inf. Model.*, **2021**, 61 (10), 5234-5242, doi: 10.1021/acs.jcim.1c00897
7. Zhang, S; Vayer, M.; Noël, F.; Vuković, V.D.; Golushko, A.; **Rezajooei, N.**; **Rowley, C.N.**; Leboeuf, D.; Moran J. Unlocking the Friedel–Crafts Arylation of Primary Aliphatic Alcohols and Epoxides Driven by Hexafluoroisopropanol *Chem* **2021**, 7, 2245–2255, doi: 10.1016/j.chempr.2021.10.023
8. Chatelain, P., Muller, C., Sau, A, Brykczynska, D., **Bahadori, M**, **Rowley, C.N.**, Moran, J. Desulfonative Suzuki-Miyaura Coupling of Sulfonyl Fluorides *Angew. Chem. Int. Ed. Engl.*, **2021**, 60, 25307–25312, doi: 10.1002/anie.202111977
9. **Lahey S.-L. J.**, **Phuc, Tu**, **Rowley, C. N.**, Benchmarking Force Field and the ANI Neural Network Potentials for the Torsional Potential Energy Surface of Biaryl Drug Fragments *J. Chem. Inf. Model*, **2020**, 60 (12), 6258–6268, doi: 10.1021/acs.jcim.0c00904
10. **Mohebifar M.**, **Rowley C. N.**, An Efficient and Accurate Model for Water with an Improved Non-Bonded Potential, *J. Chem. Phys.* **2020**, 153, 134105, doi: 10.1063/5.0014469
11. Vant, J., **Lahey, S-L. J.**, Jana, K., Shekhar, M., Sarkar, D., Munk, B. H., Kleinekathöfer, U., Mittal, S., **Rowley, C. N.**, Singharoy, A. Flexible fitting of small-molecules into electron microscopy maps using molecular dynamics simulations with Neural Network Potentials, *J. Chem. Inf. Model.*, special issue on Frontiers in CryoEM Modeling, doi: 10.1021/acs.jcim.9b01167

12. **Lahey S.-L. J.**, **Rowley, C. N.**, Simulating Protein–Ligand Binding with Neural Network Potentials *Chem. Sci.*, **2020**, doi: 10.1039/C9SC06017K
13. Sandeep Inakollu, V. S., Geerke, D. P., **Rowley, C. N.**, Yu, H., Polarisable force fields: What do they add in biomolecular simulations? *Curr. Opin. Struct. Biol.*, doi: 10.1016/j.sbi.2019.12.012, invited review
14. Chatelain, P., Sau, A., **Rowley, C. N.**, Moran, J. The Suzuki–Miyaura Coupling of Arylsulfones, *Angew. Chem. Int. Ed.*, **2019**, 58 (42), 14959-14963 doi: 10.1002/anie.201908336
15. **Awoonor-Williams, E**; Isley III, W; Dale, S; Roux, B; Becke, A; Yu, H; Johnson, E. R.; Rowley, C. N. Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols, *J. Comput. Chem.*, **2019**, doi: 10.1002/jcc.26064
16. Jackman, K. M. K., Bridge, B. J., Sauvé, E. R., **Rowley, C.N.**, Zheng, C. H. M., Stubbs, J. M., Boyle, P. D., Blacquiere, J. M., C(sp3)–C(sp3) Coupling with a Pd(II) Complex Bearing a Structurally Responsive Ligand *Organometallics* **2019** doi: 10.1021/acs.organomet.9b00014
17. Raycroft, M. A. R., Racine, K. E., **Rowley, C. N.**, Keillor, J. W., Mechanisms of Alkyl and Aryl Thiol Addition to N-methylmaleimide *J. Org. Chem.* **2018**, doi: 10.1021/acs.joc.8b01638
18. **Awoonor-Williams, E.**, **Rowley, C. N.** How Reactive are Druggable Cysteines in Protein Kinases? *J. Chem. Inf. Model.* **2018**, doi: 10.1021/acs.jcim.8b00454
19. **Awoonor-Williams, E.**, **Rowley, C. N.** The Hydration Structure of Methylthiolate from QM/MM Molecular Dynamics *J. Chem. Phys.* **2018**, 149, 045103 doi: 10.1063/1.5038010
20. Richmond, E., Yi, J., Vuković, V. D., **Sajadi, F.**, **Rowley, C. N.**, Moran, J., Ring-opening hydroarylation of monosubstituted cyclopropanes enabled by hexafluoroisopropanol. *Chem. Sci.* **2018**, doi: 10.1039/C8SC02126K
21. Hazel, A., Walters, E., **Rowley, C. N.**, Gumbart, J.C. Folding free energy landscapes of β-sheets with non-polarizable and polarizable CHARMM force fields *J. Chem. Phys.* **2018**, 149, 072317, doi: 10.1063/1.5025951
22. **Walters, E.**, **Mohebifar, M.**, Johnson, E.R., **Rowley, C. N.**, Evaluating the London Dispersion Coefficients of Protein Force Fields Using the Exchange-Hole Dipole Moment Model, *J. Phys. Chem. B.* **2018**, doi: 10.1021/acs.jpcb.8b02814
23. **Mohebifar, M.**, Johnson, E. R., **Rowley, C. N.**, Evaluating Force-Field London Dispersion Coefficients Using the Exchange-Hole Dipole Moment Model, *J. Chem. Theory Comput.* **2017** doi: 10.21/acs.jctc.7b00522
24. **Awoonor-Williams, E., Walsh, A. G., Rowley, C. N**. Modeling Covalent-Modifier Drugs, *BBA – Proteins and Proteom.*, **2017**, doi: 10.1016/j.bbapap.2017.05.009, invited review
25. **Awoonor-Williams, E., Rowley, C. N.** The Hydration Structure of Carbon Monoxide by Ab Initio Methods, *J. Chem. Phys.* **2017**, doi: 10.1063/1.4974164, (preprint)
26. **Gaalswyk, K., Awoonor-Williams, E., Rowley, C. N.** Generalized Langevin Methods for Calculating Transmembrane Diffusivity, *J. Chem. Theory Comput.* **2016**, doi: 10.1021/acs.jctc.6b00653
27. **Awoonor-Williams, E.**, **Rowley, C. N.** Evaluation of Methods for the Calculation of the pKa of Cysteine Residues in Proteins, *J. Chem. Theory Comput.* **2016**, doi: 10.1021/acs.jctc.6b00631
28. **Gaalswyk, K., Rowley, C.N.** An explicit-solvent conformation search method using open software *PeerJ* **2016**, doi: 10.7717/peerj.2088
29. Lee, C., Comer, J., Herndon, C., Leung, N; Pavlova, A., Swift, R., Tung, **Rowley, C.N.**, Amaro, R; Chipot, C., Wang, Y., Gumbart, J. Simulation-based approaches for determining membrane permeability of small compounds *J. Chem. Inf. Model.* **2016** doi: 10.1021/acs.jcim.6b00022

30. **Awoonor-Williams, E., Rowley C.N.** Molecular Simulation of Non-facilitated Membrane Permeation, *Biochim. Biophys. Acta - Biomembranes*, **2016**, 1672–1687, doi: 10.1016/j.bbamem.2015.12.014, invited review
31. **Adluri, A, Murphy, J. N, Tozer, T. Rowley C.N.** A Polarizable Force Field with a Sigma-Hole for Liquid and Aqueous Bromomethane. *J. Phys. Chem. B* **2015**, *119* (42), 13422–13432, doi: 10.1021/acs.jpcb.5b09041
32. **Smith, J.M., Rowley, C.N.** Automated Computational Screening of the Thiol Reactivity of Substituted Alkenes, *J. Comput. Aided Mol. Design* **2015**, 29 (8), 725–735 doi: 10.1007/s10822-015-9857-0
33. **Riahi, S., Rowley C.N.** Why Can Hydrogen Sulfide Permeate Cell Membranes? *J. Am. Chem. Soc.* **2014**, 136 (43), 15111–15113, doi: 10.1021/ja508063s
34. Yi, L., **Rowley, C.N.**, Kerton, F. Combined experimental and computational studies on the physical and chemical properties of the renewable amide, 3-acetamido-5-acetylfuran. *ChemPhysChem*, **2014**, 15, 4087–4094, doi: 10.1002/cphc.201402376
35. **Riahi, S., Rowley C.N.** The CHARMM-TURBOMOLE Interface for Efficient and Accurate QM/MM Molecular Dynamics, Free Energies, and Excited State Properties. *J. Comput. Chem.* **2014**, 35 (28), 2076–2086, doi: 10.1002/jcc.23716
36. **Hickey, A. L., Rowley, C.N.**Benchmarking Quantum Chemical Methods for the Calculation of Molecular Dipole Moments and Polarizabilities. *J. Phys. Chem. A*, **2014**, 118 (20), 3678–3687 doi: 10.1021/jp502475e
37. **Riahi, S**., **Rowley, C.N.** Solvation of Hydrogen Sulfide in Liquid Water and at the Water/Vapor Interface Using a Polarizable Force Field, *J. Phys. Chem. B*, **2014**, 118 (5), 1373–1380, doi: 10.1021/jp4096198
38. **Smith, J.M., Jami Alahmadi, Y., Rowley, C.N.**, Range-Separated DFT Functionals are Necessary to Model Thio-Michael Additions, *J. Chem. Theory Comput.* **2013** 9 (11), 4860–4865, doi: 10.1021/ct400773k
39. Jurca, T., **Hiscock, L.K.**, Korobkov, I. **Rowley, C.N.**, Richeson, D.S. The Tipping Point of the Inert Pair Effect: Experimental and Computational Comparison of In(I) and Sn(II) bis(imino)pyridine Complexes, *Dalton Trans.* **2015**, 43, 690–697 doi: 10.1039/c3dt52227j
40. **Rowley, C.N.**, Roux, B. A computational study of barium blockades in the KcsA potassium channel based on multi-ion potential of mean force calculations and free energy perturbation, *J. Gen. Physiol.*, **2013**, doi: 10.1085/jgp.201311049
41. **Riahi, S., Rowley, C.N.** A Drude Polarizable Force Field for Liquid Hydrogen Sulfide *J. Phys. Chem. B* **2013** 117 (17), 5222–5229 doi: 10.1021/jp401847s
42. Riahi, S., Roux, B., Rowley, C.N. QM/MM Molecular Dynamics Simulations of the Hydration of Mg(II) and Zn(II) Ions. *Can. J. Chem.* **2013** 91 (7), 552–558, special issue in honour of Dennis Salahub
43. Li, J., Pandelieva, A.T., Rowley, C.N., Woo, T.K., Wisner, J.A. Importance of Secondary Interactions in Twisted Doubly Hydrogen Bonded Complexes. *Org. Lett.*, **2012** 14 (22), 5772–5775

Prior to Appointment

41. **Rowley, C.N**., Roux, B. The Solvation Structure of Na^+ and K^+ in Liquid Water Determined from High Level ab Initio Molecular Dynamics Simulations *J. Chem. Theory Comput.*, **2012**, 8 (10), 3526–3535, doi: 10.1021/ct300091w

42. Roux, B., Bernéche, S., Egwolf, B., Lev, B., Noskov, S.Y., **Rowley, C.N.**, Yu, H. Ion Selectivity in Channels and Transporters. *J. Gen. Physiol.,* 137 (5) 415–426, 2011

43. **Rowley, C.N.**, Woo, T.K.Counteranion Effects on the Zirconocene Polymerization Catalyst Olefin Complex from QM/MM Molecular Dynamics Simulations. *Organometallics*, 30(8), 2071–2074, 2011

44. **Rowley, C.N.**, Woo, T.K. New Shooting Algorithms for Transition Path Sampling: Centering Moves and Varied Perturbation Sizes for Improved Sampling. *J. Chem. Phys.*, 131, 234102, 2009

45. Tam, R.Y., **Rowley, C.N.**, Petrov, I., Zhang, T., Afagh, N.A., Woo, T.K., Ben, R.N., Solution Conformation of C-Linked Antifreeze Glycoprotein Analogues and Modulation of Ice Recrystallization. *J. Am. Chem. Soc.*, 131 (43), 15745–15753, 2009

46. **Rowley, C.N.**, Woo, T.K. Computational design of ruthenium hydride olefin-hydrogenation catalysts containing hemilabile ligands. *Can. J. Chem.,* 87 (7), 1030–1038, 2009, special issue in honour of Tom Ziegler

47. **Rowley, C.N.**, Mosey, N.J., Woo, T.K. A Computational Experiment of the endo vs. exo Preference in a Diels-Alder Reaction. *J. Chem. Ed.*, 86 (2), 199–201, 2009

48. **Rowley, C.N.**, Woo, T.K. Reaction Dynamics of β-Hydrogen Transfer in the Zirconocene Olefin Polymerization Catalyst: A DFT Path Sampling Study. *Organometallics*, 27 (24), 6405–6407, 2008

49. **Rowley, C.N.**, Ong, T.-G., Priem, J. Richeson, D., Woo, T. K. Analysis of the Critical Step in Catalytic Carbodiimide Transformation: Proton Transfer from Amines, Phosphines, and Alkynes to Guanidinates, Phosphaguanidinates, and Propiolamidinates with Li and Al Catalysts. *Inorg. Chem.*, 47(24), 12024–12031, 2008

50. **Rowley, C.N.**, van der Eide, E.F., Piers, W.E.; Woo, T.K. DFT Study of the Isomerization and Spectroscopic/Structural Properties of Ruthenacyclobutane Intermediates Relevant to Olefin Metathesis. *Organometallics*, 27 (23), 6043–6045, 2008

51. **Rowley, C.N.**, Ong, T.-G. Priem, J., Richeson, D., Woo, T.K. Amidolithium and Amidoaluminum Catalyzed Synthesis of Substituted Guanidines: An Interplay of DFT Modeling and Experiment. *Inorg. Chem.*, 47 (20), 9660–9668, 2008

52. **Rowley, C.N.**, Woo, T.K. A Path Sampling Study of Ru-Hydride Catalyzed H_2-Hydrogenation of Ethylene. *J. Am. Chem. Soc.*, 130 (23), 7218–7219, 2008

53. Dornan, P., **Rowley, C.N.**, Priem, J., Barry, S.T., Woo, T.K. Richeson, D.S. Atom Efficient Cyclotrimerization of Dimethylcyanamide Catalyzed by Aluminium Amide: A Combined Experimental and Theoretical Investigation. *Chem. Commun.* 3645–3647, 2008

54. **Rowley, C.N.**, Foucault, H.M., Woo, T.K.; Fogg, D.E. Mechanism of Olefin Hydrogenation Catalyzed by $RuHCl(L)(PR)_3)_2$ Complexes (L = CO, PR_3: A DFT Study. *Organometallics*, 27 (8), 1661–1663, 2008

55. **Rowley, C.N.**, Woo, T.K. Generation of initial trajectories for transition path sampling of chemical reactions with ab initio molecular dynamics. *J. Chem. Phys.*, 126, 024110–024118, 2007

56. Lafrance, M., **Rowley, C.N.**,Woo, T.K., Fagnou, K. Catalytic Intermolecular Direct Arylation of Perfluorobenzenes. *J. Am. Chem. Soc.* 128, 8754–8756, 2007

57. Brazeau, A.L., Wang, Z., **Rowley, C.N.**, Barry, S.T. Synthesis and Thermolysis of Aluminum Amidinates: A Ligand-Exchange Route for New Mixed-Ligand Systems. *Inorg. Chem.*, 45 (5), 2276–2281, 2006

58. **Rowley, C.N.**, DiLabio, G.A., and Barry, S.T. Theoretical and Synthetic Investigations of Carbodiimide Insertions into Al-$N(CH_3)_2$ Bonds. *Inorg. Chem.*, 44 (6), 1983–1991, 2005

59. Wright, J.S., **Rowley, C.N.**, and Chepelev, L.L. A "universal" B3LYP-based method for gas-phase molecular dissociation enthalpy, ionization potential, electron and proton gas phase acidity. *Mol. Phys.* 103, (6–8), 815–823, 2005

Book Chapters

E. Awoonor-Williams, **J. Kennedy**, **C.N. Rowley**, Measuring and Predicting Warhead and Residue Reactivity, Annual Reports in Medicinal Chemistry *The Design of Covalent-Based Inhibitors* Volume 56. Eds: Richard Ward, Neil Grimster, Academic Press, **2020**

Presentations

Invited Talks

1. NAMD Workshop, Chicago IL, U.S.A., August 9–10, 2022
2. Tinker Workshop, Bethesda MD, U.S.A., June 2–-4, 2022
3. WATOC 2022 - Vancouver BC, July 3–8, 2022
4. CCCE 2022, Symposium in Memory of Sergei Noskov, Calgary AB, 2022
5. Targeted Covalent Inhibition: Review of the Field and Recent Advances, American Chemical Society National Meeting, March 31, 2019, Orlando, USA
6. Molecular Mechanical Force Fields with Higher-order Dispersion Terms Using the Exchange-hole Dipole Moment Model, American Chemical Society National Meeting, Free Energy Methods and Membrane Proteins Session, August 19–-23, 2018, Boston, MA
7. Including Higher-Order Dispersion in Molecular Mechanical Force Fields, 28th Canadian Symposium on Theoretical and Computational Chemistry, July 19, 2018, Windsor, ON, Canada
8. Solvation of Thiolates from QM/MM Molecular Dynamics, 101th Canadian Society for Chemistry Conference, Edmonton AB, May 31, 2018 Membrane Permeability of Gasotransmitters from Multi-scale Modeling, 101th
9. Canadian Society for Chemistry Conference, Edmonton AB, May 31, 2018 Including Higher-Order Dispersion in Molecular Mechanical Force Fields, 101th Canadian Society for Chemistry Conference, Edmonton AB, May 29, 2018
10. Modeling Covalent Modifier Drugs, Beyond K_d's: New computational methods to address challenges in drug discovery, June 6, 2017 to June 9, 2017, Location: CECAM-HQ-EPFL, Lausanne, Switzerland
11. Generalized Langevin Methods for Calculating Transmembrane Diffusivity, 99th Canadian Society for Chemistry Conference, June 6, 2016, Session in Honour of Benoît Roux
12. Modelling Biophysical Chemistry with High Performance Computing, High Performance Computing Symposium 2014, June 27, 2014, Halifax, NS, Canada
13. Fast and Accurate QM/MM Molecular Dynamics Using CHARMM-TURBOMOLE, June 4, 2014, Multi-scale Computational Approaches and Applications in Biochemistry and Biomaterials Symposium of the Physical, Theoretical and Computational Chemistry Division, 97th Canadian Chemistry Conference and Exhibition, Vancouver, BC, Canada
14. Towards a Polarizable Force Field for Modeling Petroleum Desulfurization. ACS 245th National Meeting, April 10, 2013

15. Interpreting Barium Blockade Kinetics of Potassium Channels Using Multi-Ion Potential of Mean Force Calculations, 25th Canadian Symposium on Theoretical and Computational Chemistry, Guelph, ON, July 26, 2012
16. High Level QM/MM Molecular Dynamics Simulations of Ion Solvation, 95th Canadian Chemistry Conference and Exhibition, Calgary, AB, Canada, May 27, 2012

Departmental Seminars

1. University of Windsor, January 20, 2020
2. University of Strasbourg, Strasbourg, France, 2019
3. Center for Molecular Modeling, University of Ghent, Ghent, Belgium, June 21, 2019
4. University of Saarland, Saarbrucken, Germany, 2019
5. Department of Chemistry, Technical University of Munich, Munich, Germany, 2019
6. Department of Chemistry, Universidad de Concepción, Concepción, Chile, January 24, 2019
7. Department of Chemistry, Universidad Andrés Bello, Santiago, Chile, January 22, 2019
8. Department of Chemistry,University of Wollongong, Australia, January 19, 2019
9. Department of Chemistry,University of Hawaii at Manoa, Honolulu, Hawaii, USA, January 12, 2019
10. Department of Chemistry, University of Lethbridge, Lethbridge AB, November 9, 2018
11. Department of Chemistry, University of Calgary, Calgary AB, November 7, 2018
12. Department of Chemistry, Dalhousie University, Halifax NS, September 28, 2018
13. Department of Chemistry, University of British Columbia – Okanagan, Department of Chemistry, September 25, 2018
14. Department of Chemistry, York University, Toronto ON, September 19, 2018
15. Department of Pharmacy, Western University of Health Sciences, Pomona, CA, USA, August 15, 2017
16. Departments of Chemistry and Physics, Georgia Institute of Technology, Atlanta, GA, USA, August 17, 2017
17. Department of Chemistry, Queen's University, April 7, 2017
18. Department of Chemistry, Memorial University of Newfoundland, February 4, 2016
19. Department of Chemistry and Biomolecular Science, University of Ottawa, October 21, 2015
20. Department of Chemistry, Carleton University, October 19, 2015
21. Inorganic Chemistry Group, University of Wurzburg, Wurzburg, Germany, July 16, 2015
22. Department of Chemistry and Biochemistry, Concordia University, April 9, 2015
23. Department of Chemistry, Wilfrid Laurier University, December 12, 2014
24. Department of Chemistry, University of New Brunswick, October 24, 2014 (Science Atlantic tour)
25. Department of Chemistry, Mount Allison University, NB, October 23, 2014 (Science Atlantic tour)
26. Department of Chemistry, University of Prince Edward Island, PE, October 22, 2014 (Science Atlantic tour)
27. Department of Chemistry, University of Manitoba, Winnipeg, MB, September 26, 2014
28. Department of Chemistry, Acadia University, Wolfville, NS, June 24, 2014
29. Department of Chemistry, Cape Breton University, Sydney, NS, June 23, 2014

30. University of California - Merced, Merced, CA, USA, February 14, 2014
31. Memorial University of Newfoundland, St. John's, NL, November 1, 2013
32. Departments of Chemistry and Physics, St. Francis Xavier University, October 4, 2013
33. Department of Chemistry, St. Mary's University, Halifax, NS, Canada, April 29, 2013

Conference Organization

1. Session in Honour of Benoît Roux and Computational Biophysical Chemistry Session, 2016 Canadian Society for Chemistry Conference Session Co-organizer (with Professor Guillaume Lamoureux)
2. Computational and Theoretical Chemistry Symposium, 2015 Canadian Society for Chemistry Conference Session Co-organizer (with Professor Nick Mosey)
3. 2014 Memorial University Biophysics Symposium (October 4, 2014) Conference chair and lead organizer
4. Chemistry Undergraduate Poster Session, Lead organizer, August 17, 2012
5. 13th Atlantic Theoretical Chemistry Symposium (August 3–4, 2013)

Funding

1. NSERC Discovery Grant
    - Computational Methods for Modeling Drug Kinetics, Term: 2019–2024, Total Amount: $240,000
    - Development and Application of New Tools for Computational Biophysical Chemistry, Term: 2012–2018, Total Amount: $228,000
2. RDC Ignite R&D, Computational Modeling of Ionic Liquid Extraction of Sulfur Contaminants from Crude Oil, Term: 2012–2014, Total Amount: $95,037

Awards to Students

1. Phuc Tu, H. Bernstein Memorial Award, 2022, $4086
2. Ernest Awoonor-Williams, 2022 CAS Future Scholar
3. Ernest Awoonor-Williams, 2017–2020, $50000 p.a.
4. Ernest Awoonor-Williams, NSERC Vanier Scholarship, 2017–2020, $50000 p.a.
5. Ernest Awoonor-Williams, NSERC Vanier Scholarship, 2017–2020, $50000 p.a.
6. Ernest Awoonor-Williams, Best Oral Presentation in Physical Chemistry, Science Atlantic ChemCon 2017
7. Archita Adluri, CIC Poster Award, Science Atlantic ChemCon 2017, $100
8. Ernest Awoonor-Williams, ACENET Fellowship (graduate), 2016, $10000
9. Ernest Awoonor-Williams, A. G. Hatcher, Scholarship, 2015, $15000
10. Ernest Awoonor-Williams, ACEmat Award for Best Talk at Science Atlantic ChemCon, 2015, $50
11. Ernest Awoonor-Williams, ACENET Fellowship (graduate), 2015, $10000
12. Jessica Besaw, Alexander Graham Bell Canada Graduate Scholarship (doctoral), 2015, $35,000 p.a. (3 years)
13. Jessica Besaw, A. G. Hatcher Scholarship, 2014, $15000
14. Jessica Besaw, Biophysical Society of Canada Travel Award

15. Jessica Besaw, 2014 Memorial University Biochemistry Symposium, 1st runner up, August 13, 2014
16. Jessica Besaw, Outstanding Student Presentation Award, 97th Canadian Chemistry Conference and Exhibition, Vancouver, BC, June 5, 2014
17. Jennifer M. Smith, Award in the Physical, Theoretical and Computational Chemistry Division Poster Presentation, 97th Canadian Chemistry Conference and Exhibition, Vancouver, BC, June 3, 2014
18. Saleh Riahi, J. Beryl Truscott Graduate Scholarship, 2013, $2000

Service

International

1. National Academy of Sciences (USA) Proposal Evaluation for Allocation of Supercomputing Time for the Study of Molecular Dynamics Simulations 2016–2018

National

1. Canada Foundation for Innovation (CFI) Merit Review Committee for drug discovery/development.
2. Organizer for the CSC Physical, Theoretical, and Computational online seminars, 2020–present
3. NSERC Discovery Grant Evaluation Group (1504 - Chemistry), 2019–2022
4. Compute Canada Research Allocation Committee, Biophysics, Chemistry, and Biochemistry, 2012–2016
5. Co-organizer, Session in Honour of Benoît Roux, 99th Canadian Society for Chemistry Conference
6. Co-organizer of Computational Chemistry Symposium, 98th Canadian Society for Chemistry Conference

Institutional

1. Research Committee, 2021–present, Department of Chemistry, Carleton University
2. Chair selection committee, Department of Chemistry, Carleton University
3. Graduate Studies Committee, 2012–2018, Department of Chemistry, Memorial University
4. Graduate Recruiting Committee, 2014–2018, Department of Chemistry, Memorial University
5. Headship Search Committee, 2015, Department of Chemistry, Memorial University
6. Canada Research Chair Search Committee, 2016–2017, Department of Chemistry, Memorial University
7. Physical Chemistry Search Committee (chair), Department of Chemistry, Memorial University
8. NSERC CGS-M selection committee, 2014–present, Memorial University
9. Board of Study, Scientific Computing Program, 2014–present, Memorial University

Graduate Supervision

1. Maryam Bahadori, 2021–present, Ph.D. (chemistry), Carleton University
2. Sheyla Montero, 2019–2022, M.Sc. (biochemistry), Memorial University of Newfoundland, Ph.D. (biochemistry) Carleton University
3. Tu Nguyen Thien Phuc, 2021–present, Ph.D. (chemistry), Carleton University
4. Victor Hugo Cano Gill, 2021–present, Ph.D. (chemistry), Carleton University
5. Nazanin Rezajooei, 2019–2022, M.Sc. (scientific computing, co-op option), Memorial University of Newfoundland
6. Shae-Lynn Lahey, 2019–2022, M.Sc. (chemistry), Memorial University of Newfoundland
7. Ernest Awoonor-Williams, 2014–2020, Ph.D (chemistry), Memorial University of Newfoundland, NSERC Vanier Scholar
8. Mohamad Mohebifar, 2016–2018, M.Sc. (chemistry), Memorial University of Newfoundland
9. Fatemeh Sajadi, 2016–2018, M.Sc. (chemistry), Memorial University of Newfoundland
10. Kari Gaalswyk, 2014–2016, M.Sc. (scientific computing), Memorial University of Newfoundland
11. Jessica Besaw, 2013–2015, M.Sc. (chemistry), Memorial University of Newfoundland
12. Saleh Riahi, 2012–2014, M.Sc. (chemistry), Memorial University of Newfoundland

Teaching

1. Quantum Chemsitry (CHEM 3101), 2021
2. Methods of Computational Chemistry (CHEM 3102), 2021–2022
3. Computational Chemistry Laboratory (CHEM 3106), 2021–2022
4. Statistical Thermodynamics and Rate Theories (CHEM 3303), 2012–2020
5. Advanced Statistical Thermodynamics (CHEM 4305), 2012–2019
6. Scientific Programming (CMSC 6920), 2014–2017
7. General Chemistry (CHEM 1050), 2015–2016