Nicholas Mosey

Associate Professor and Graduate Chair
Department of Chemistry
Queen's University
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OVERVIEW

- Associate Professor of Chemistry
- Research interests: Computational and theoretical chemistry; friction, wear and lubrication; density functional theory; molecular dynamics
- Teaching: General chemistry; quantum chemistry; computational chemistry; numerical methods; scientific leadership

APPOINTMENTS

Associate Professor of Chemistry 2014-present
Assistant Professor of Chemistry 2008-2014
Department of Chemistry, Queen's University

- Using first-principles chemical simulations to gain atomic-level insights into the processes responsible for friction and wear
- Development of analytical models connecting atomic-level phenomena to real-world properties of interested in industrial and technological applications
- Development of improved chemical simulation methods, with an emphasis on extending the time scales accessible in molecular dynamics simulations of reactions and incorporating exact exchange into calculations of periodic systems

NSERC Postdoctoral Fellow 2006-2008
Department of Mechanical and Aerospace Engineering, Princeton University
Supervisor: Emily Carter

- Developed predictive multi-scale simulation models linking the atomic-level details of transition metal oxides to their macroscopic properties
- Developed first-principles methods for performing electronic structure calculations of strongly correlated electron materials
- Investigated the mechanical failure of transition metal oxides using quantum chemistry
- Funded by NSERC Postdoctoral Fellowship and awarded Howard Alper Award as top Canadian NSERC PDF

EDUCATION

PhD Theoretical Chemistry and Scientific Computing 2001-2006

Department of Chemistry, University of Western Ontario

"Formation and Function of Zinc Dialkyldithiophosphate Engine Anti-Wear Films: Molecular-Level Insight through Chemical Simulation"
Thesis advisor: Tom Woo

- Used quantum chemical methods to investigate the anti-wear functionality of motor oil additives, ultimately leading to a new model of wear inhibition
- Developed methods to extend the time scales accessible in *ab initio* molecular dynamics simulations
- Research generated new commercial sponsorship from General Motors, Conoco-Phillips and British Petroleum
- Recognized as top PhD thesis in science in Canada in 2006

BSc Honors Chemistry 1997-2001

Department of Chemistry, University of Western Ontario

Research advisor: Tom Woo

FUNDING

11. Natural Science and Engineering Research Council of Canada: Discovery Frontiers Grant, 2015-2019 ($4,000,000).
10. Compute Canada National Research Allocation Competition, 2014-2016 ($235,000).
9. Natural Sciences and Engineering Research Council of Canada: Discovery Grant, 2011-2015 ($350,000).
8. Xerox Research Centre of Canada: University Partnership Grant, 2011-2012 ($24,000).
7. Natural Sciences and Engineering Research Council of Canada: CREATE Grant, 2010-2015 ($1,568,500).
6. Ontario Ministry of Research and Innovation: Early Researcher Award, 2009-2014 ($150,000).
5. Natural Sciences and Engineering Council of Canada: Undergraduate Student Research Awards Program, 2009, 2011, 2013 ($13,500).
4. Queen's University: Principal's Development Fund, 2009 ($6,800).
3. Queen's University: Summer Work Experience Program, 2008-2009 ($23,520).
2. Natural Sciences and Engineering Research Council of Canada: Discovery Grant, 2008-2010 ($146,400).
1. Queen's Research Initiation Grant, 2008 ($110,000).

AWARDS AND HONOURS

14. Graduating Class Award for Excellence in Teaching Chemistry, 2016.
13. Graduating Class Award for Excellence in Teaching Chemistry, 2014.
12. Frank Knox Teaching Award Nominee, 2012.
11. W.J. Barnes Teaching Excellence Award Nominee, 2010.
10. Ontario Council of Universities John Charles Polanyi Prize, 2009, ($20,000).
9. Ontario Ministry of Innovation Early Researcher Award, 2009-2014.
8. Natural Science and Engineering Research Council of Canada (NSERC) Postdoctoral Fellowship, 2006-2008, ($80,000).
7. NSERC Doctoral Prize, 2007, ($10,000) [Top Canadian Ph.D. thesis in the natural sciences].
6. Howard Alper Postdoctoral Prize, 2006, ($20,000) [Top NSERC Postdoctoral Fellowship applicant across all scientific and engineering disciplines].
5. Paul de Mayo Award, 2006, ($2,500) [Top Ph.D. thesis in the Department of Chemistry at the University of Western Ontario].
4. NSERC Canada Graduate Scholarship, 2004-2006, ($105,000).
3. Robert and Ruth Lumsden Fellowship in Science, 2004, ($2,000).
2. NSERC Post Graduate Scholarship, 2002-2004, ($45,000).
1. Christian Sivertz Scholarship in Physical Chemistry, 2002, ($2,500).

TRAINING

Current students

6. Soran Jahangiri, PDF (2014 – current)
5. Yaoting Zhang, Ph.D. student (2012 – current)
4. Laura Laverdure, Ph.D. student (2015 – current)
3. Mathew Neal, M.Sc. student (2014 – current)
2. Chloe Graham, B.Sc. thesis student (2016 – current)
1. Hannah Taylor, B.Sc. thesis student (2016 – current)

Former students

30. Gavin Heverly-Coulson, PDF (2012 – 2014)
29. Prakash Dayal, PDF (2010 – 2014)
28. Hongjuan Zhu, PDF (2010 – 2011)

27. Gurpaul Kochhar, Ph.D. student (2011 – 2016), M.Sc. student (2009 – 2011)
26. Chris Maxwell, Ph.D. student (2009 – 2012)
25. Stephanie Whyte, M.Sc. student (2012 – 2015)
24. Carolyn Carkner, M.Sc. student (2011 – 2013), summer student (2009, 2010)
23. Adrian Bailey, M.Sc. student (2010 – 2011), summer student (2009)
22. Ben Carver, M.Sc. student (2008 – 2010), research assistant (2010 – 2012)
21. Joseph Willemsen, B.Sc. thesis student (2015 – 2016), summer student (2016)
20. Jeff Mountjoy, summer student (2013, 2014)
19. Adam Hall, thesis student (2013 – 2014), NSERC USRA (2014)
18. Alex Ford, thesis student (2013 – 2014)
17. Matthew Pacchione, thesis student (2012 – 2013)
16. Michael Kilgour, thesis student (2012 – 2013)
15. Michelle Todd, thesis student (2012 – 2013)
14. Justin Brooks, B.Sc. thesis student (2011 – 2012)
13. Steven Brooks, B.Sc. thesis student (2011 – 2012)
12. Julie Sischek, B.Sc. thesis student (2011 – 2012)
11. Leanne Chen, NSERC USRA (2011)
10. Jamie Evans, B.Sc. thesis student (2010 – 2011), summer student (2011)
9. Robert Lee, B.Sc. thesis student (2010 – 2011), summer student (2011)
8. Julie Winterburn, B.Sc. thesis student (2010 – 2011)
7. Faisal Abdullah, B.Sc. thesis student (2009 – 2010)
6. Sarah Haw, B.Sc. thesis student (2009 – 2010)
5. Jason Beischlag, summer student (2009)
4. Chris Carr, B.Sc. thesis student (2008 – 2009)
3. Sabine Weyand, B.Sc thesis student (2008 – 2009)
2. Joanne McNeish, summer student (2008)
1. Grant Pettypiece, summer student (2008)

PUBLICATIONS

66. Jahangiri, S.; Mosey, N.J., "Theoretical Investigation of Magnesium Hydroxide and Calcium Hydroxide Nanostructures." *Physical Chemistry Chemical Physics*, submitted.

65. Mountjoy, J.; Todd, M.; Mosey, N.J., "Exact Exchange with Non-Orthogonal Generalized Wannier Functions." *Journal of Chemical Physics*, submitted.

64. Jahangiri, S.; Mosey, N.J., "Theoretical Insights into the Friction Coefficients of Layered Materials: Impact of van der Waals Interactions, Sliding Directions, Heterolayers, and Absorbed Species." *Physical Review B*, submitted.

63. Zhang, Y., Mosey, N.J., "High Pressure Chemistry of Thioaldehydes: A First-Principles Molecular Dynamics Study." *Journal of Chemical Physics*, in press.

62. Kochhar, G.S.; Mosey, N.J., "Differences in the Abilities to Mechanically Eliminate Activation Energies for Unimolecular and Bimolecular Reactions." *Nature Scientific Reports*, **2016**, *6*, 23059.

61. Crudden C.M.; Horton J.H.; Narouz M.R.; Smith C.A.; Li Z.; Munro K.; Baddeley C.J.; Larrea C.R.; Drevniok B.; Thanabalasingam B.; McLean A.B; Zenkina O.V.; Ebralidze I.I.; She Z.; Kraatz H.B.; Mosey N.J.; Saunders L.N.; Yagi A., "Bio-Sensing with Robust, Readily Formed, Self-Assembled Carbene Monolayers on Gold." *Nature Communications*, **2016**, *7*, 12654.

60. Jahangiri S.; Heverly-Coulson G,; Mosey N.J., "The Development and Assessment of Atomistic Models for Predicting Static Friction Coefficients." *Physical Review B*, **2016**, *94*, 075406.

59. Ang M.T.C.; Phan L.; Alshamrani A.K.; Harjani J.R.; Wang R.Y.; Schatte G.; Mosey N.J.; Jessop P.G., "Contrasting Reactivity of CS_2 with Cyclic vs. Acyclic Amidines." *European Journal of Organic Chemistry*, **2015**, *33*, 7334.

58. Wu N.; Melan C.F.C.; Stevenson, F.O.; Guo H.; Habib F.; Holmberg R.F.; Murugesu M.; Mosey N.J.; Nierengarten H.; Petitjean A., "Systematic Study of the Synthesis and Coordination of 2-(1,2,3-triazol-4-yl)-Pyridine to Fe(II), Ni(II) and Zn(II); Ion-Induced Folding into Helicates, Mesocates and Larger Architectures, and Application to Magnetism and Self-Selection." *Dalton Transactions*, **2015**, *44*, 14991.

57. Manzhos S.; Carrington Jr. T.; Laverdure L.; Mosey N.J., "Computing the Anharmonic Vibrational Spectrum of UF_6 in 15 Dimensions with an Optimized Basis Set and Rectangular Collocation." *Journal of Physical Chemistry A*, **2015**, *119*, 9557.

56. Kochhar G.S.; Heverly-Coulson G.; Mosey N.J., "Theoretical Approaches for Understanding the Interplay between Stress and Chemical Reactivity." *Polymer Chemistry*, **2015**, *37*, 369.

55. Whyte S.M.; Mosey N.J., "Behavior of Two-Dimensional Hydrogen-Bonded Networks Under Shear Conditions: A First-Principles Molecular Dynamics Study." *Journal of Physical Chemistry C*, **2015**, *119*, 350.

54. Thompson M.; Carkner C.J.; Mosey N.J.; Kapernaum N.; Lemieux R.P., "Tuning the mesomorphic properties of phenoxy-terminated smectic liquid crystals – the effect of fluoro substitution." *Soft Matter*, **2014**, *11*, 3860.

53. Thompson M.; Carkner C.J.; Bailey A.; Mosey N.J.; Kapernaum N.; Lemieux R.P., "Tuning the mesogenic properties of 5-alkoxy-2-(4-alkoxyphenyl)pyrimidine liquid crystals: the effect of a phenoxy end-group in two sterically equivalent series." *Liquid Crystals*, **2014**, *9*, 1246.

52. Maxwell C.I.; Neverov A.A.; Mosey N.J.; Brown R.S., "Density Functional Theory Study of Methoxide Promoted and Zn(II)-Complexed Methoxide Promoted Cleavages of Aryl- and Alkyl Acetates in Methanol. Transition From Concerted to Stepwise Processes as a Function of Leaving Group Ability." *Journal of Physical Organic Chemistry*, **2014**, *24*, 419.

51. Crudden C.; Horton J.; Ebralidze I.; Zenkina O.; Keske E.; Leake J.; Rousina-Webb A.; MacLean A.; Drevniok B.; Seki T.; Wu G.; Mosey N.J., "Ultra-Stable Self-Asembled Monolayers of N-Heterocyclic Carbenes on Gold." *Nature Chemistry*, **2014**, *6*, 409.

50. Rao Y.; Amarne H.; Chen L.; Brown M.; Mosey N.J.; Wang S., "Photo- and Thermal-Induced Multistructural Transformation of 2-Phenylazolyl Chelate Boron Compounds." *Journal of the American Chemical Society*, **2013**, *135*, 3407.

49. Maxwell C.I.; Mosey N.J.; Brown, R.S., "DFT Computational Study of the Methanolytic Cleavage of DNA and RNA Phosphodiester Models Promoted by the Dinuclear Zn-(II) Complex of 1,3-Bis(1,5,9-triazacyclododec-1-yl)propane." *Journal of the American Chemical Society*, **2013**, *135*, 17209.

48. Yan Y.; Zhao W.; Bhagavathy G.; Faurie A.; Mosey N.J.; Petitjean A., "Controlled Synthesis and Alkaline Earth Ion Binding of Switchable Formamidoxime-Based Crown Ether Analogs." *Chemical Communications*, **2012**, *48*, 7829.

47. Rao, Y.-L.; Chen, L.D.; Mosey, N.J.; Wang. S., "Stepwise Intramolecular Photoisomerization of NHC-Chelate Dimesitylboron Compounds with C-C Bond Formation and C-H Bond Insertion." *Journal of the American Chemical Society*, **2012**, *134*, 11026.

46. Akhshi, P.; Mosey, N.J.; Wu, G., "Free-Energy Landscapes of Ion Movement through G-Quadruplex Channel." *Angewandte Chemie International Edition*, **2012**, *51*, 2850.

45. Maxwell, C.I.; Liu, C.T.; Neverov, A.A.; Mosey, N.J.; Brown, R.S., "Transition from Concerted to Stepwise Processes as a Function of Leaving Group Ability: Density Functional Theory and Experimental Study of Lyoxide-Promoted Cleavages of Phosphorothioate and Phosphate Triesters in Water and Methanol." *Journal of Physical Organic Chemistry*, **2012**, *25*, 437.

44. Edwards, D.R.; Maxwell, C.I.; Harkness, R.W.; Neverov, A.A.; Mosey, N.J.; Brown, R.S., "Experimental and Computational Determination of Bronsted Coefficients for Equilibrium Transfer of the O,O-Dimethyl Phosphorothioyl Group between Oxyanion Nucleophiles." *Journal of Physical Organic Chemistry*, **2012**, *25*, 258.

43. Haw, S.M.; Mosey, N.J., "Tribochemistry of Aldehydes Sheared between (0001) Surfaces of α-Alumina from First-Principles Molecular Dynamics." *Journal of Physical Chemistry C*, **2012**, *116*, 2132.

42. Bailey, A.; Mosey, N.J., "Prediction of Reaction Barriers and Force-Induced Instabilities under Mechanochemical Conditions with a Parameterized Model: A Case Study of the Ring Opening of 1,3-Cyclohexadiene." *Journal of Chemical Physics*, **2012**, *136*, 044102.

41. Zhu, H.; Mosey, N.J., "The Tensile Strengths of Heterogeneous Interfaces: A Comparison of Static and Dynamic First-Principles Calculations." *Journal of Chemical Physics*, **2011**, *135*, 244706.

40. Liu, C.T.; Maxwell, C.I.; Pipe, S.G.; Neverov, A.A.; Mosey, N.J.; Brown, R.S., "Methanolysis of Thioamide Promoted by a Simple Palladacycle is Accelerated by 10^8 over the Methoxide Catalyzed Reaction." *Journal of the American Chemical Society*, **2011**, *133*, 20068.

39. Dayal, P.; Weyand, S.A.; McNeish, J.; Mosey, N.J., "Temporal Quantum Mechanics / Molecular Mechanics: Extending the Time Scales of Molecular Dynamics Simulations of Reactions." *Chemical Physics Letters*, **2011**, *516*, 263.

38. Zhao, W.; Wang, R.; Mosey, N.J.; Petitjean, A., "Alkoxyamine-derived Formamidines: Configurational Control and Molecular Folding." *Organic Letters*, **2011**, *13*, 5160.

37. Capela, M.; Mosey, N.J.; Xing, L.; Wang, R.; Petitjean, A., "Amine Exchange in Formamidines." *Chemistry - A European Journal*, **2011**, *17*, 4598.

36. Haw, S.M.; Mosey, N.J., "Chemical Response of Aldehydes to Compression between (0001) Surfaces of Alumina." *Journal of Chemical Physics*, **2011**, *134*, 014702.

35. Bissesur, R.; Loppnow, G.; Mosey, N.J.; Carran, J.; Chik, J. "Chemistry: Student Activity, Chemical Reactivity Workbook." Nelson Education, Toronto (2011).

34. Liu, C.T.; Maxwell, C.I.; Neverov, A.A.; Mosey, N.J.; Brown, R.S., "Mechanistic and Computational Study of Palladacycle-Catalyzed Decomposition of a Series of Neutral Phosphorothioate Triesters in Methanol." *Journal of the American Chemical Society*, **2010**, *132*, 16599.

33. Tian, Z.; Stairs, R.A.; Mosey, N.J.; Dust, J.M.; Kraft, T.M.; Buncel, E., "Spirooxazine to Merooxazine Interconversion in the Presence and Absence of Zinc. Approach to a Bistable Photochemical Switch." *Journal of Physical Chemistry A*, **2010**, *114*, 11900.

32. Carkner, C.J.; Mosey, N.J., "Slip Mechanisms of Hydroxylated Al_2O_3 (0001)/(0001) Interfaces: A First-Principles Molecular Dynamics Study." *Journal of Physical Chemistry C*, **2010**, *114*, 17709.

31. Kochhar, G.S.; Bailey, A.; Mosey, N.J., "Competition between Orbitals and Stress in Mechanochemistry." *Angewandte Chemie International Edition*, **2010**, *49*, 7452.

30. Carkner, C.J.; Haw, S.M.; Mosey, N.J.., "Effect of Adhesive Interactions on Static Friction at the Atomic Scale." *Physical Review Letters*, **2010**, *105*, 056102.

29. Mosey, N.J., "Compression-Induced Polymerization of Aldehydes: A Quantum Chemical Study." *Journal of Chemical Physics*, **2010**, *132*, 134513.

28. Mosey, N.J.; Carter, E.A., "Shear Strength of Chromia across Multiple Length Scales: an LDA+U Study." *Acta Materialia*, **2009**, *57*, 2933.

27. Shakhvorostov, D.; Muser, M.H.; Mosey, N.J.; Song, Y.; Norton, P.R., "Correlating Cation Coordination, Stiffness, Phase Transition Pressures and Smart Materials Behavior in Metal Phosphates." *Physical Review B*, **2009**, *79*, 094107.

26. Mosey, N.J.; Carter, E.A., "*Ab initio* LDA+U Prediction of the Tensile Properties of Chromia across Multiple Length Scales." *Journal of the Mechanics and Physics of Solids*, **2009**, *57*, 287.

25. Rowley, C.N.; Mosey, N.J.; Woo, T.K., "A Computational Experiment of the endo versus exo Preference in a Diels-Alder Reaction." *Journal of Chemical Education*, **2009**, *86*, 199.

24. MacQuarrie, S.; Thompson, M.; Blanc, A.; Mosey, N.J.; Lemieux, R.P.; Crudden, C.M., "Chiral Mesoporous Organosilicates based on Axially Chiral Monomers." *Journal of the American Chemical Society*, **2008**, *130*, 14099.

23. Mosey, N.J.; Liao, P.; Carter, E.A., "Rotationally-Invariant *ab initio* Evaluation of Exchange and Coulomb Parameters for DFT+U Calculations." *Journal of Chemical Physics*, **2008**, *129*, 014103.

22. Shakvorostov, D.; Muser, M.H.; Mosey, N.J.; Munoz-Paniagua, D.J.; Pereira, G.; Song, Y.; Norton, P.R., "On the Pressure-Induced Amorphization of Zinc Phosphates." *Journal of Chemical Physics*, **2008**, *128*, 074706.

21. Mosey, N.J.; Carter, E.A., "*Ab initio* Evaluation of Coulomb and Exchange Parameters for DFT+U Calculations." *Physical Review B*, **2007**, *76*, 155123.

20. Zhu, J.; Mosey, N.J.; Woo, T.K.; Huang, Y., "A Study of the Adsorption of Toluene in Zeolite LiNa-Y by Solid-State NMR Spectroscopy." *Journal of Physical Chemistry C*, **2007**, *111*, 13427.

19. Mosey, N.J.; Muser, M.H. "Atomistic Modeling of Friction." Reviews in Computational Chemistry. K.B. Lipkowitz, R. Larter, T.R. Cundari, Eds. Wiley-VCH, New York, 2007, Vol. 25, pp 67-124.

18. Lacey, D.; Hu, X.K.; Loboda, A.V.; Mosey, N.J.; Lipson, R.H., "Aspirin Revealed: A Strategy for Detecting Acetylsalicylic Acid by MALDI Mass Spectrometry." *International Journal of Mass Spectrometry*, **2007**, *261*, 192.

17. Mosey, N.J.; Woo, T.K. "Computational Catalyst Design: An Introduction and Overview of Current Technologies." Advanced Catalyst Design II. The Catalyst Group Resources, Inc., Sprint House, PA, 2006, pp 45-85.

16. Mosey, N.J.; Woo, T.K.; Kasrai, M.; Norton, P.R.; Bancroft, G.M.; Muser, M.H., "Interpretation of Experiments on ZDDP Anti-Wear Additives and Films through Pressure-Induced Cross-Linking." *Tribology Letters*, **2006**, *24*, 105.

15. Nistor, R.; Polihronov, J.G.; Muser, M.H.; Mosey, N.J., "A Generalization of the Charge Equilibration Method for Non-Metallic Materials." *Journal of Chemical Physics*, **2006**, *125*, 094108.

14. Mosey, N.J.; Woo, T.K., "An *ab initio* Molecular Dynamics and Density Functional Theory Study of the Formation of Phosphate Chains from Metathiophosphates." *Inorganic Chemistry*, **2006**, *45*, 7464.

13. Mosey, N.J.; Woo, T.K., "Insights into the Chemical Nature of Zinc Dialkyldithiophosphates in their Isomeric and Decomposed Forms through Molecular Simulation." *Tribology International*, **2006**, *39*, 979.

12. Wanapun, D.; Van Gorp, K.A.; Mosey, N.J.; Kerr, M.A.; Woo, T.K., "The Mechanism of 1,3-Dipolar Cycloaddition Reactions of Cyclopropanes and Nitrones: A Theoretical Study." *Canadian Journal of Chemistry*, **2005**, *83*, 1752.

11. Mosey, N.J.; Muser, M.H.; Woo, T.K. "Molecular Mechanisms of Anti-Wear Pad Formation and Functionality." *Proceedings of the World Tribology Congress III*, **2005**, *3*, 63954.

10. Mosey, N.J.; Woo, T.K.; Muser, M.H. "Mechanisms of Wear Inhibition by ZDDP Lubricant Additives - Insights from Molecular Scale Simulations." *Preprints of the American Chemical Society Division of Petroleum Chemistry*, **2005**, *50*, 332.

9. Mosey, N.J.; Woo, T.K.; Muser, M.H. "Rational Design of New Anti-Wear Additives for Engine Lubricants through Molecular Simulation." *Preprints of the American Chemical Society Division of Petroleum Chemistry*, **2005**, *50*, 291.

8. Mosey, N.J.; Woo, T.K., "Formation of Zinc Phosphate Polymers and Networks through the Insertion of Metathiophosphates into Zinc Dialkyldithiophosphates." *Inorganic Chemistry*, **2005**, *44*, 7274.

7. Mosey, N.J.; Woo, T.K.; Muser, M.H., "Energy Dissipation via Quantum Chemical Hysteresis during High-Pressure Compression: A First-Principles Molecular Dynamics Study of Phosphates." *Physical Review B*, **2005**, *72*, 054124.

6. Mosey, N.J.; Muser, M.H.; Woo, T.K., "Molecular Mechanisms for the Functionality of Lubricant Additives." *Science*, **2005**, *307*, 1612.

5. Lam, S.; Shi, Y.J.; Mosey, N.J.; Woo, T.K.; Lipson, R.H., "Mechanisms for the Formation of Gas-Phase Protonated Alcohol-Ether Adducts by VUV Laser Ionization and Density Functional Calculations." *Journal of Chemical Physics*, **2004**, *121*, 1612.

4. Mosey, N.J.; Woo, T.K., "A Quantum Chemical Study of the Unimolecular Decomposition Reactions of Zinc Dialkyldithiophosphate Anti-Wear Additives." *Journal of Physical Chemistry A*, **2004**, *108*, 6001.

3. Mosey, N.J.; Woo, T.K., "The Finite Temperature Structure and Dynamics of Zinc Dialkyldithiophosphate Wear Inhibitors: a Density Functional Theory and *ab initio* Molecular Dynamics Study." *Journal of Physical Chemistry A*, **2003**, *107*, 5058.

2. Mosey, N.J.; Hu, A.; Woo, T.K., "*ab initio* Molecular Dynamics Simulations with a HOMO-LUMO Gap Biasing Potential to Accelerate Rare Reaction Events." *Chemical Physics Letters*, **2003**, *373*, 498.

1. Mosey, N.J.; Baines, K.M.; Woo, T.K., "Mechanism of the Addition of Nonenolizable Aldehydes and Ketones to (Di)metallenes: A Density Functional and Multiconfigurational Perturbation Theory Study." *Journal of the American Chemical Society*, **2002**, *124*, 13306.

INVITED PRESENTATIONS

29. Mosey, N.J., "*Slipping and Sliding First-Principles Simulations of Tribological Processes.*" Queen's University, Department of Physics Colloquium. Kingston, ON, Canada. (2016).

28. Mosey, N.J., "*Slipping and Sliding First-Principles Simulations of Tribological Processes.*" Concordia University, Department of Chemistry and Biochemistry Seminar Series. Montreal, QC, Canada. (2016).

27. Mosey, N.J., "*Slipping and Sliding First-Principles Simulations of Tribological Processes.*" Quantum Systems in Chemistry, Physics, and Biology (QSCP-XXI). Vancouver, BC, Canada. (2016). (plenary lecture)

26. Mosey, N.J., "*Slipping and Sliding First-Principles Simulations of Tribological Processes.*" 99^{th} Canadian Chemistry Conference and Exhibition. Ottawa, ON, Canada. (2016).

25. Mosey, N.J., "*First-Principles Simulations of Tribological Processes.*" Center for Molecular Simulation Seminar Series. Calgary, AB, Canada. (2016).

24. Mosey, N.J., "*Tribological Behaviour of 2D Hydrogen-Bonded Networks.*" 97^{th} Canadian Chemistry Conference and Exhibition. Ottawa, ON, Canada. (2015).

23. Mosey, N.J., "*Temporal QM/MM: Extending the Time-Scales of MD Simulations of Reactions*" 96^{th} Canadian Chemistry Conference and Exhibition. Vancouver, BC, Canada. (2014).

22. Mosey, N.J., " *Computational Chemistry: Methods, Applications and Opportunities*" Queen's Graduate Computing Society Conference. Kingston, ON, Canada. (2014). (keynote lecture)

21. Mosey, N.J., "*First-Principles Simulations of Tribological Processes.*" Afton Chemicals Research Seminar Series. Richmond, Virginia, US. (2013).

20. Mosey, N.J., "*First-Principles Simulations of Tribological Processes.*" University of Victoria Department of Chemistry Seminar Series. Victoria, BC, Canada. (2013).

19. Mosey, N.J., "*Effects of Mechanical Stress on Electronic Structure and Energy.*" 95^{th} Canadian Chemistry Conference and Exhibition. Quebec City, QC, Canada. (2013).

18. Mosey, N.J., "*First-Principles Simulations of Tribological Processes.*" Dalhousie University Department of Chemistry Seminar Series. Halifax, NS, Canada. (2013).

17. Mosey, N.J., "*Inducing Chemical Reactions Through Applied Stress.*" 95^{th} Canadian Chemistry Conference and Exhibition. Calgary, AB, Canada. (2012).

16. Mosey, N.J., "*First-Principles Simulations of Tribochemical Reactions.*" 12^{th} Annual CERMM Symposium. Montreal, QC, Canada. (2012).

15. Mosey, N.J., "*First-Principles Simulations of Tribochemical Reactions.*" University of Ottawa Department of Chemistry Seminar Series. Ottawa, ON, Canada. (2012).

14. Mosey, N.J., "*First-Principles Simulations of Tribochemical Reactions.*" Cape Breton University Department of Chemistry Seminar Series, Sydney, NS, Canada. (2011).

13. Mosey, N.J., "*Inducing Chemical Reactions Through Applied Stress.*" Atlantic Theoretical Chemistry Symposium. Charlottetown, PEI, Canada. (2011). (plenary lecture)

12. Mosey, N.J., "*Quantum Chemical Simulations of Tribochemical Reactions.*" Trent University, Chemistry/Physics Seminar Series. Peterborough, Ontario, Canada. (2011).

11. Mosey, N.J., "*Quantum Chemical Simulations of Tribochemical Reactions.*" 2010 International Chemical Congress of Pacific Basin Societies (Pacifichem). Honolulu, HI, USA. (2010).

10. Mosey, N.J., "*Extending the Laws of Friction to Account for Chemical Interactions within Sliding Contacts.*" 26$^{\text{th}}$ Symposium on Chemical Physics. Waterloo, ON, Canada. (2010).

9. Mosey, N.J., "*First-Principles Simulations of Tribological Processes.*" 17$^{\text{th}}$ Canadian Symposium on Theoretical Chemistry. Edmonton, AB, Canada. (2010).

8. Mosey, N.J., "*First Principles Simulations of Tribological Processes.*" Xerox Research Centre of Canada Invited Speaker Seminar Series. Mississauga, ON, Canada. (2010).

7. Mosey, N.J., "*Extending the Time-Scales Accessible in Molecular Dynamics Simulations of Chemical Reactions.*" 93$^{\text{rd}}$ Canadian Chemistry Conference and Exhibition. Toronto, ON, Canada. (2010).

6. Mosey, N.J., "*Quantum Chemical Simulations of Tribochemical Processes.*" ExxonMobil Products, Research & Technology Center. Paulsboro, NJ, USA. (2010).

5. Mosey, N.J., "*Inducing Chemical Reactions through Applied Stress.*" University of Toronto Chemical Physics Colloquium. Toronto, ON, Canada. (2010).

4. Mosey, N.J, Liao, P., Carter, E.A., "*First-Principles Evaluation of Coulomb and Exchange Parameters for DFT+U Calculations.*" Sixth Congress of the International Society for Theoretical Chemical Physics. Vancouver, BC, Canada. (2008).

3. Mosey, N.J., Carter, E.A., "*Development of First-Principles Cohesive Laws for Strongly-Correlated Electron Materials.*" 90$^{\text{th}}$ Canadian Chemistry Conference and Exhibition. Winnipeg, MB, Canada. (2007).

2. Mosey, N.J., "*Accurate Evaluation of the Electronic and Mechanical Properties of Transition Metal Oxides – Towards a Predictive Multiscale Model of Wear.*" Paul de Mayo Award Lecture, University of Western Ontario, London, ON, Canada. (2007).

1. Mosey, N.J., "*Modeling Fatigue and Wear of Strongly-Correlated Electron Materials.*" PICASso Computational Lecture Series, Princeton University. Princeton, NJ, USA. (2007).

TEACHING

Queen's University (2008 – present):

- CHEM 112: General Chemistry
- APSC 132: Chemistry and it's Applications
- CHEM 313: Introduction to Quantum Mechanics
- CHEM 346: Quantum Mechanics and Chemical Simulation
- CHEM 413: Computational Chemistry

- CHEM 834: Computational Chemistry
- CHEM 838: Numerical Methods in Chemistry
- CHEM 938: Density Functional Theory

Princeton University (2006 – 2008):

- MAE 324: Structures and Properties of Materials (substitute lecturer)
- APC 509: Concepts in Electronic Structure Theory (substitute lecturer)

University of Western Ontario (2004):

- CHEM 374: Introduction to Quantum Mechanics (substitute lecturer)

Course Development
Queen's University:

- CHEM 113/114: Online Version of CHEM 112: General Chemistry (2014)
- CHEM 904: Scientific Leadership (2016)

Course Coordination
Queen's University:

- CHEM 112: General Chemistry (2013, 2016)
- CHEM 904: Scientific Leadership (2017)

COMMITTEES

Positions within the Department of Chemistry at Queen's University

- Graduate Coordinator (2011 – present)
- Curriculum and Programs Super-Committee (co-chair: 2012 – 2016)
- Organizational Super-Committee (co-chair: 2012 – 2016)
- Graduate Committee (member: 2008 – 2010, chair: 2011 – present)
- Graduate Awards Committee (member: 2008 – 2010, chair: 2011 – present)
- Graduate Admissions Committee (chair: 2011 – present)
- Graduate Recruitment Committee (chair: 2011 – 2013)
- Graduate Curriculum Committee (2011 – present)
- Instructional Assignment Committee (2011 – present)
- TA Assignment Committee (member: 2012 – 2014, chair: 2016 – present)
- Timetabling Committee (2012 – present)

- Renewal, Tenure and Promotion Committee (2009)
- Head Selection Committee (2011/2012, 2016/2017)
- CHEM 112 Blended Learning Development Committee (2012 – 2013)
- First-Year Curriculum Reform Committee (member: 2010, chair: 2016)
- Information Technology Committee (2009 – 2011)
- Computer Resources and Website Committee (2012 – 2014)
- Student Relations Committee (2012 – 2013)

Positions within Queen's University, but External to the Department of Chemistry

- Faculty of Arts and Science Graduate Council (member: 2011 – present, associate chair: 2013 – 2014, 2016 – present)
- Graduate Fellowships Committee (2012 – present)
- Graduate Funding Committee (2013 – 2014)
- Entrance Awards Reviewer (2010 – present)

Positions external to Queen's University

- Ontario Graduate Scholarship Adjudication Panel (2012)
- NSERC Discovery Grant Reviewer (2011 – present)
- NSF Grant Reviewer (2012 – 2013)
- ACS Petroleum Research Fund Grant Reviewer (2010)