Curriculum Vitae

Paul W. Ayers

January 31, 2017

Personal Background:

Born May 2, 1974; Greenville, North Carolina, United States of America

Educational Background:

Undergraduate (1992-1996): David Lipscomb University (Nashville, Tennessee, U.S.A.)
- **Degree:** B.S.; Summa Cum Laude (4.0 G.P.A.)
- **Majors:** Physics; Chemistry (mathematics emphasis); Mathematics (physics emphasis)

Graduate (1996-2001): Department of Chemistry; The University of North Carolina at Chapel Hill (U.S.A.)
- **Degree:** Ph.D. in Chemistry
- **Division:** Physical Chemistry
- **Major Professors:** Robert G. Parr (primary) and Max L. Berkowitz

Postdoctoral Associate (2001-2002): Department of Chemistry; Duke University (U.S.A.)
- **Supervisor:** Weitao Yang
- **Fellowships:** National Institutes of Health Postdoctoral Research Fellowship

Employment History:

Assistant Prof. (2002-2007): Department of Chemistry & Chemical Biology; McMaster University
Associate Prof. (2007-2013): Department of Chemistry & Chemical Biology; McMaster University
Professor (2013-present): Department of Chemistry & Chemical Biology; McMaster University

Awards & Other Recognition

Canada Research Chair in Theoretical Chemistry and Chemical Biology (Tier 2) (2002-2012)
Wiley International Journal of Quantum Chemistry Award (2002)
Research Innovation Award (Research Corp.) (2004)
Premier's Research Excellence Award (Ontario Government) (2004)
Alfred P. Sloan Fellowship (2008-2010)
Keith Laidler Award (Canadian Society for Chemistry; "for distinguished contribution to the field of physical chemistry while working in Canada. The award recognizes early achievement in the awardees independent research career.") (2011)
Dirac Medal (World Association of Theoretically Oriented Chemists; "for the outstanding theoretical and computational chemist in the world under the age of 40") (2012)
Annual Medal of the International Academy of Quantum Molecular Science ("to a young member of the scientific community who has distinguished himself/herself by a pioneering and important contribution") (2012)
E. W. R. Steacie Memorial Fellowship ("to highly promising university faculty who are earning a strong international reputation for original research") (2013-2015)
Steacie Prize for Natural Sciences ("top Canadian scientist or engineer aged 40 or younger") (2013)
Rutherford Memorial Medal in Chemistry from the Royal Society of Canada ("for outstanding research in chemistry") (2014)
2014 Promising Scientist Award of the Centre de Mécanique Ondulatoire Appliquée (CMOA)
University Scholar (McMaster University) (2015-present)
Canada Research Chair in Theoretical Chemistry (Tier 1) (2016-)
Elected to the College of Young Scholars of the Royal Society of Canada (2016)

Biographical Information

Despite the fact—or maybe *because*—my parents are chemistry professors, I came to science relatively late. Growing up in rural Eastern North Carolina (U.S.A.), I did high school internships in management and architecture before eventually deciding to become a writer. It was late in my senior year of high school—and after I had applied to a smorgasbord of liberal arts colleges—that I decided to study physics. This led me to Lipscomb University (which was the only university I'd applied to with a decent physics program). I began my undergraduate studies in 1992 and soon realized that I enjoyed the mathematical aspects of physics more than applications. So I added mathematics as a second major. After my second year at university, one of my parents' colleagues (Robert Morrison; East Carolina Univ.) hired me to do summer research in theoretical chemistry. This was a transformative experience: I learned that I could use the tools I love (mathematics and physics) to study problems I find interesting (how and why chemical reactions happen). So I added chemistry as a third major. After two more years of diligent study (and one more summer of research, this time in a collaborative project between chemistry (Prof. Morrison) and physics (Prof. Orville Day)), I graduated in 1996 with a triple-major in mathematics, physics, and chemistry (and a perfect 4.0 G.P.A.). I also took nearly twenty elective courses in philosophy, theology, and creative writing, reflecting broad interests that I maintain to this day.

Based partly on the generous fellowship support from the University of North Carolina (Venable, Reilley, and Kenan fellowships; I won an NSF fellowship a year later), I opted to pursue a Ph.D. in chemistry under the direction of Prof. Robert Parr. Working with Prof. Parr was a second transformative experience. Prof. Parr's approach to research—using mathematics and physics to study fundamental problems in chemistry and chemical reactivity—appealed to me, and soon I was "addicted" to research. Upon receiving my Ph.D. in 2001, I fed this addiction by joining the research group of Weitao Yang in the chemistry department at Duke University (where I was supported by a postdoctoral fellowship from the National Institutes of Health). While Prof. Yang's research also uses physics and mathematics at a high level, his research focuses on developing new computational methods for biochemistry and materials' science. With Prof. Yang, I learned more about computational methods and the ways theoretical chemistry can be used to address practical problems. My postdoctoral experience completed my transformation from mathematical physics to my current research niche, which lies somewhere between Prof. Parr (whose research is typically more abstract) and Prof. Yang (whose research is typically more applied).

After one year with Prof. Yang, I left to become an assistant professor of chemistry at McMaster University, where I held the Canada Research Chair in Theoretical Chemistry and Chemical Biology from 2002 to 2012. Since arriving at McMaster, I have focused on establishing my career as a teacher (my teaching evaluations are consistently among the best in the department) and a researcher. In the latter capacity, I have published the usual complement of book chapters (20 published or in press) and scientific papers (215 published or accepted); I have given 185 invited presentations at conferences and universities around the world. I have also established an international network of collaborators, ranging from mathematical chemists (e.g., Prof. Mel Levy, Tulane Univ. (emeritus)) to applied computational chemists (e.g., the Center for Molecular Modeling, Ghent Univ.).

This record of accomplishment has been recognized with the Wiley International Journal of Quantum Chemistry Award, a Research Innovation Award (from Research Corporation, 2004), a Premier's Research Excellence Award (from the Ontario government, 2004), an Alfred P. Sloan fellowship (2008), the Keith Laidler Award (from the Canadian Society for Chemistry, 2011), the Dirac Medal (from the World Association of Theoretically Oriented Chemists, 2012), the annual medal of the International Academy of Quantum Molecular Science (2012), an E. W. R. Steacie Jr. Fellowship (from the National Sciences and Engineering Research Council (NSERC) of Canada, 2013), the Steacie Prize (2013), the Rutherford Medal (from the Royal Society of Canada, 2014), and the Promising Scientist Award (from the Centre de Mécanique Ondulatoire Appliquée, 2014).

1. Research Interests

My research focuses on developing new mathematical and computational tools for describing and predicting chemical processes, especially chemical reactions. Studying how chemical bonds fracture and form requires understanding how the electrons that bind atoms into molecules rearrange during chemical reactions and, more subtly, how different molecular environments influence these rearrangements. Thus, theoretical methods for modeling chemical reactions belong to the realm of electronic structure theory, or quantum chemistry. Within the broad purview of quantum chemistry, my research focuses on:

- qualitative tools for understanding chemical reactivity
- quantitative tools for predicting chemical reaction mechanisms
- accurate and efficient approaches to the underlying electronic structure problem.

Qualitative tools provide essential guidance for choosing which experiments and computations are likely to give interesting results and provide an intuitive framework for understanding results and designing follow-up studies. My work on qualitative tools for predicting chemical reactivity has been based on density-functional theory (DFT); this approach permits the derivation of *qualitative* principles from *exact* theory through a process of systematic and controlled approximation. (By contrast, in molecular-orbital theory or valence-bond theory, qualitatively-useful models correspond to quantitatively-inaccurate calculations.) When I started working on DFT reactivity theory, the formal development was based either on the analogy to classical thermodynamics or the analogy to perturbation theory in quantum mechanics. In my Ph.D. work, I formulated a third approach, based on variational principles.[2,3] Many workers in this field are currently working to develop new external potential-based reactivity tools, where changes in external potential (e.g., the number, type, and location of atomic nuclei) are used to probe molecules' reactivity. Reference 3 is often regarded as the foundational paper for this area of research. Recently, I have been working to explain classical reactivity tools and to develop new tools for cases where classical reactivity paradigms fail. For example, I proposed the "redox induced electron transfer" effect (wherein oxidation of a molecule is coupled to the reduction of the atom in the molecule, or vice versa) prior to the surge of experimental activity in this area.[11] I have also worked to elucidate the foundations of classical precepts like the hard/soft acid/base principle[7,12] and the Woodward-Hoffmann rules.[13] My current focus is on density-based population analysis[8] and energy decomposition analysis.[16] I like these approaches because they clearly delineate the contributions from overlap/Pauli, charge-transfer, and polarization effects. Because the electron density is the only required input, these techniques are easily extended to correlated wavefunctions. One can even envision using these tools to analyze the results of orbital and basis-set free *ab initio* methods like quantum Monte Carlo.

After qualitative tools have been used to winnow the list of possibilities, one needs a quantitative tool for predicting the chemical reaction mechanism of the process(es) of interest. My work in this area has focused on applying the fast-marching method to the problem of determining chemical reaction paths.[4,6] The key insight is that the problem of finding chemical reaction paths on complicated potential energy surfaces can be written as a static Hamilton-Jacobi equation. This equation then is solved using an efficient "front-growing" algorithm called the fast-marching method. The great advantage of this approach is its universality (very complicated potential energy surfaces can be explored) and its parallelizability (by exploiting the analogy to wavefront propagation). Currently we are developing new computational methods that use some of the same "tricks" (cost functions, dimensional partitioning, etc.) as the fast-marching approach, but which are more computationally efficient.[18,20] These enhanced methods are being used to study diverse systems, from gas-phase isomerizations to enzymatic catalysis. My next goal is to adapt algorithms from watershed analysis to complex reaction networks like those associated with combustion, fragmentation in mass spectrometry, and metabolism.

Both qualitative and quantitative studies of chemical reactivity require information about the electronic structure of the molecules in question. This motivates my work on developing more accurate and efficient quantum chemistry methods. Throughout my career, most of my research in electronic structure theory has focused on DFT, primarily at a formal and algorithmic[15] level. More recently, I have been interested in the extensions and generalizations of DFT. Recognizing the importance of faster computations, my first work in this direction explored whether functions that were even simpler than the electron density might suffice to determine all of the properties of molecular systems. While that work was successful at a formal level,[1] it does not seem practical to me. (Others disagree.) More recently, I have studied nonlocal exchange-correlation energy functionals and generalizations of conventional DFT, wherein one constructs a hierarchy of "generalized" density-functional theories based on descriptors that contain more information than the electron density.[9] Most of my work has focused on the k-electron distribution functions (k=1 is the normal electron density; k=2 is the electron pair density).[5,10] Together with my European collaborators, I studied approaches based on the k-electron reduced density matrices (k-RDM). We demonstrated that the usual variational approaches based on the 2-RDM are not size-consistent and do not possess a derivative discontinuity for integer electron number; these effects combine to give qualitatively absurd results for dissociating molecules (and other failures).[17] These problems can be fixed[19] by enforcing stronger N-representability conditions (like the "sharp P" and "sharp Q" conditions I had previously derived[14])

or by using "wavefunction information" to induce a derivative discontinuity (as in Kohn-Sham DFT). Arguably the biggest problem is the computational inefficiency of these methods; one of my graduate students is preparing to address this issue. My main focus now is using the wavefunction-forms of exactly solvable model Hamiltonians for quantum chemistry. Because these wavefunctions are based on real model systems, they capture the key qualitative effects of electron correlation; because the models are exactly solvable, the methods are computationally facile. The numerical results are very promising, often within a few microHartree of benchmark quantum chemistry methods. In addition, this approach has resolved several old formal problems. (E.g., by these methods we discovered the first computationally practical antisymmetric product of nonorthogonal geminals, a wavefunction ansatz that was proposed by leading theorist like Pauling, Fock, Pople, Lennard-Jones, and Hurley around 1950 but discarded due to its computational expense and mathematical intricacy.)[21,22]

1. 2000 (Ayers) "Density Per Particle as a Descriptor of Coulomb Systems." *Proc. Natl. Acad. Sci. USA*, 97:1959.
2. 2000 (Ayers, Parr). "Variational Principles for Site Selectivity in Chemical Reactivity: The Fukui Function and Chemical Hardness Revisited." *J. Am. Chem. Soc.* 122:2010.
3. 2001 (Ayers, Parr). "Variational Principles for Describing Chemical Reactions: Reactivity Indices Based on the External Potential." *J. Am. Chem. Soc.* 123:2007.
4. 2004 (Dey, Janicki, Ayers). "Hamilton-Jacobi Equation for the Least Action/Least Time Dynamical Path Based on the Fast-Marching Method" *J. Chem. Phys.*, 121:6667.
5. 2005 (Ayers) "Generalized Density Functional Theories Using the *k*-electron Densities: Development of Kinetic-Energy Functionals." *J. Math. Phys.* 45:062107.
6. 2005 (Dey, Ayers) "A Generalized Hamilton-Jacobi Equation for Computing Minimum Potential Energy Paths." *Mol. Phys.* 104:541.
7. 2005 (Ayers) "An elementary derivation of the hard/soft acid/base principle"; *J. Chem. Phys.*, *Communication* **122**, 141102.
8. 2005 (Parr, Ayers, Nalewajski) "What Is An Atom in A Molecule"; *J. Phys. Chem. A* 109:3957.
9. 2006 (Ayers, Golden, Levy). "Generalizations of the Hohenberg-Kohn theorem." *J. Chem. Phys.*, 124:054101.
10. 2006 (Ayers). "Using the Classical Many-Body Structure to Determine Electronic Structure: An Approach Using k-electron Distribution Functions." *Phys. Rev. A*, 74:042502.
11. 2006 (Ayers). "Can One Oxidize an Atom by Reducing the Molecule that Contains It?" *PCCP*, 8:3387.
12. 2007 (Ayers). "The Physical Basis of the Hard/Soft Acid/Base Principle." *Far. Disc.*, 135:161.
13. 2007 (Ayers, Morell, De Proft, Geerlings) "Understanding the Woodward-Hoffmann Rules Using Changes in the Electron Density. (No Orbitals Necessary.)" *Chemistry, A European Journal*, 13:8240.
14. 2007 (Van Neck, Ayers). "Necessary Conditions for the *N*-representability of the Second-Order Reduced Density Matrix: Upper Bounds on the P and Q Matrices." *Phys. Rev. A*, 75:032502.
15. 2008 (Rodriguez, Thompson, Ayers, Köster), "Numerical Integration of Exchange-Correlation Energies and Potentials Using Transformed Sparse Grids." *J. Chem. Phys.* 128:224103
16. 2009 (Wu, Ayers, Zhang) "Density-based energy decomposition analysis for intermolecular interactions with variationally optimized intermediate state energies." *J. Chem. Phys.*, 131:164112.
17. 2009 (Van Aggelen, Bultinck, Verstichel, Van Neck, Ayers). "Incorrect Diatomic Dissociation in Variational Reduced Density Matrix Theory Arises from the Flawed Description of Fractionally Charged Atoms." *PCCP-Communication*, 11:5558.
18. 2009 (Burger, Liu, Sarkar, Ayers) "Moving Least-Squares Interpolation for the Fast-Marching and String Methods." *J. Chem. Phys.* 130:024103.
19. 2010 (Verstichel, Van Aggelen, Van Neck, Ayers, Bultinck) "Subsystem Constraints in Variational Second Order Reduced Density Matrix Optimization: Curing Size Inconsistency." *J. Chem. Phys.* 132:114113.
20. 2010 (Burger, Ayers) "Dual Grid Methods for Finding the Reaction Path on Reduced Potential Energy Surfaces." *J. Chem. Th. Comp.* 6:1490.
21. 2013 (Johnson, Ayers, Limacher, De Baerdemacker, Van Neck, Bultinck) "A Size-Consistent Approach to Strongly Correlated Systems Using a Generalized Antisymmetrized Product of Nonorthogonal Geminals." *Comput. Theoret. Chem.* 1013:101.
22. 2013 (Limacher, Ayers, Johnson, De Baerdemacker, Van Neck, Bultinck) "A new mean-field method suitable for strongly correlated electrons: computationally facile antisymmetric products of geminals." *J. Chem. Th. Comp.* 9:1394-1401.

2. RESEARCH CONTRIBUTIONS (Up-To-Date as of January 31, 2017)

2.1 Publications (Underlined authors are research trainees funded by the Ayers group. Research trainees funded by collaborators are in italics; some of these trainees are/were co-supervised)

Summary: *Google Scholar*: 9099 citations; $h = 49$; $i10 = 165$; h(last-5-years) = 34; $i10$(last-5-years) = 137.

Book Chapters (refereed unless otherwise noted):

1. Paul W. Ayers and Weitao Yang, "Density Functional Theory", in Computational Medicinal Chemistry for Drug Discovery, P. Bultinck, H. De Winter, W. Langenaeker, and J. Tollenaere, Eds., (New York, Dekker, 2003), pp. 571-616.
2. Paul W. Ayers, "Some Problems Related to Electronegativity Equalization," *Recent Progress in Computational Sciences and Engineering* in Lectures Series on Computer and Computational Sciences **4**, 1175-1177 (2005).
3. Paul W. Ayers, "Using the Electron Density as a Weight Function for Multi-Dimensional Integration," *Recent Progress in Computational Sciences and Engineering* in Lectures Series on Computer and Computational Sciences **4**, 1226-1229 (2005).
4. *T. Verstraelen*, D. Van Neck, P. W. Ayers, V. Van Speyboeck, and M. Waroquier, "The Gradient Curves Method: An Improved Strategy for the Derivation of Molecular Mechanics Valence Force Fields from *Ab Initio* Data"; *Recent Progress in Computational Sciences and Engineering* in Lectures Series on Computer and Computational Sciences **7**, 526-529 (2006).
5. Paul Geerlings, Frank De Proft, and Paul W. Ayers "Chemical Reactivity and the Shape Function," in Theoretical and Computational Chemistry, vol. 19 (*Theoretical Aspects of Chemical Reactivity*); A. Toro-Labbé, Editor (Elsevier, Amsterdam, 2007); pp. 1-26.
6. James S. M. Anderson, Juan I. Rodriguez, David C. Thompson, and Paul W. Ayers "A novel grid based approach to the electronic structure problem: Interpolants and derivatives," Quantum Chemistry Research Trends (Nova, Hauppauge NY, 2007). [not refereed]
7. Samantha Jenkins, S. R. Kirk, and Paul W. Ayers, "Topological Transitions Between Ice Phases," in Physics and Chemistry of Ice; W. F. Kuhs, Editor (Royal Society of Chemistry; Cambridge, England; 2007); pp. 249-256.
8. Samantha Jenkins, S. R. Kirk, and Paul W. Ayers, "Chemical Character of Very High Pressure Ice Phases," in Physics and Chemistry of Ice; W. F. Kuhs, Editor (Royal Society of Chemistry; Cambridge, England; 2007); pp. 257-264.
9. Samantha Jenkins, S. R. Kirk, and Paul W. Ayers, "The Importance of O-O Bonding Interactions in Various Phases of Ice," in Physics and Chemistry of Ice; W. F. Kuhs, Editor (Royal Society of Chemistry; Cambridge, England; 2007); pp. 265-272.
10. Samantha Jenkins, S. R. Kirk, and Paul W. Ayers, "Real Space Study of Mechanical Instability in Ice XI on a 'bond-by-bond' basis," in Physics and Chemistry of Ice; W. F. Kuhs, Editor (Royal Society of Chemistry; Cambridge, England; 2007); pp. 273-280.
11. Paul W. Ayers and Andrés Cedillo, "The Shape Function," in Chemical Reactivity Theory: A Density Functional View; P. Chattaraj, Editor (Taylor and Francis, Boca Raton, 2009).
12. Paul W. Ayers, Weitao Yang, and Lee Bartolotti "The Fukui Function," in Chemical Reactivity Theory: A Density Functional View; P. Chattaraj, Editor (Taylor and Francis, Boca Raton, 2009).
13. Agnes Nagy, Mel Levy, and Paul W. Ayers "Time-Independent Theories for a Single Excited State," in Chemical Reactivity Theory: A Density Functional View; P. Chattaraj, Editor (Taylor and Francis, Boca Raton, 2009).
14. Yuli Liu, Steven K. Burger, Bijoy K. Dey, Utpal Sarkar, Marek R. Janicki, and Paul W. Ayers, "The Fast Marching Method for Determining Chemical Reaction Mechanisms in Complex Systems," in Quantum Biochemistry; C. Matta, Editor (Wiley-VCH, 2010).
15. Rogelio Cuevas-Saavedra and Paul W. Ayers, "Exchange-Correlation Functionals from the Identical-Particle Ornstein-Zernike Equation: Basic Formulation and Numerical Algorithms" in Condensed Matter Theories, Vol. 25; E. V. Ludena, R. F. Bishop, and P. Iza, Editors (World Scientific, Singapore, 2011). pp. 237-249.
16. Debajit Chakraborty and Paul W. Ayers, "Derivation of Generalized von Weizsäcker Kinetic Energies from Quasiprobability Distribution Functions," in Statistical Complexity: Applications in Electronic Structure, Ed. K. Sen. (Springer, New York, 2011). pp. 35-48

17. Paul A. Johnson, Libero J. Bartolotti, Paul W. Ayers, *Tim Fievez*, and Paul Geerlings, "Charge Density and Chemical Reactivity: A Unified View from Conceptual DFT," in Modern Charge Density Analysis; C. Gatti and P. Macchi, Eds. (Springer, New York, 2012) pp. 715-764.
18. Rogelio Cuevas-Saavedra and Paul W. Ayers, "Exchange-Correlation Functionals from the Identical-Particle Ornstein-Zernike Equation: Basic Formulation and Numerical Algorithms" in Theoretical and Computational Developments in Modern Density Functional Theory; A. K. Roy, Editor (Nova Science, New York, 2012).
19. Debajit Chakraborty and Paul W. Ayers, "Kinetic energy functionals of the electron density and pair density" in Concepts and Methods in Modern Theoretical Chemistry, Volume 1: Electronic Structure and Reactivity, eds. Swapan K. Ghosh and Pratim K. Chattaraj, (CRC Press, Boca Raton, Florida, 2013), pp. 1-42.
20. Frank De Proft, Paul Geerlings, and Paul W. Ayers, "The Conceptual Density Functional Theory Perspective of Bonding," in The Chemical Bond: Fundamental Aspects of Chemical Bonding, eds. Gernot Frenking and Sason Shaik (Wiley, Darmstadt, 2014). pp. 233-270.
21. Cherif F. Matta, Ismat Sumar, Ronald Cook, and Paul W. Ayers, "Localization-Delocalization and Electron-Density-Weighted Connectivity Matrices: A Bridge Between the Quantum Theory of Atoms in Molecules and Chemical Graph Theory." In Applications of Topological Methods in Molecular Chemistry (eds. Remi Chauvin, Christine Lepetit, Bernard Silvi, Esmail Alikhani) (Springer, Berlin, 2016) pp. 53-88.
22. E. Echegaray, A. Toro-Labbe, K. Dikmenli, F. Heidar-Zadeh, N. Rabi, S. Rabi, P. W. Ayers, C. Cardenas, R. G. Parr, and J. S. M. Anderson, "Negative condensed-to-atom Fukui functions: A signature of oxidation-induced reduction of functional groups" In Correlations in Condensed Matter under Extreme Conditions (eds. G. G. N. Angilella and A. La Magna) (Springer, Berlin, 2017) pp. 259-268.
23. Ramon A. Miranda-Quintana and Paul W. Ayers, "Grand Canonical Interpolation Models" In Conceptual Density Functional Theory (accepted).
24. Ahmed A. K. Mohammed, Steven K. Burger, and Paul W. Ayers "Failures of Embedded Cluster Models for pKa Shifts Dominated by Electrostatic Effects" In Conceptual Density Functional Theory (accepted).
25. Yuli Liu and Paul W. Ayers, "Modelling Chemical Reactions with Computers" In Conceptual Density Functional Theory (accepted).
26. Farnaz Heidar-Zadeh, Paul W. Ayers, and Ramon Carbo-Dorca "A Statistical Perspective on Molecular Similarity" In Conceptual Density Functional Theory (in press).
27. Rogelio Cuevas-Saavedra, Nataly Rabi, and Paul W. Ayers, "Computing the Unconstrained Local Hardness" In Conceptual Density Functional Theory (in press).
28. Farnaz Heidar-Zadeh and Paul W. Ayers, "Molecular Similarity From Manifold Learning on D2-Property Images" In Conceptual Density Functional Theory (in press).
29. Paul W. Ayers, *Guillaume Acke*, Stijn Fias, Debajit Chakraborty, and Patrick Bultinck "A Polynomial-Scaling Algorithm for Computing the Probability of Observing Specified Numbers of Electrons in Multiple Domains Using Correlation Functions" in Theoretical & Quantum Chemistry at the Dawn of the 21st Century (ed. R. Carbó-Dorca and T. Chakraborty) Apple Academic (in press).
30. Farnaz Heidar-Zadeh and Paul W. Ayers, "Spectral Learning for Chemical Prediction" in Theoretical & Quantum Chemistry at the Dawn of the 21st Century (ed. R. Carbó-Dorca and T. Chakraborty) Apple Academic (in press).

Other:

1. Paul W. Ayers, Advances in Quantum Chemistry, Volume 48. *J. Am. Chem. Soc.* **128**, 3468-3469 (2006). [Book Review]
2. Paul W. Ayers and Gernot Frenking, "Richard Bader (1931-2012) Obituary," *Angewandte Chemie-Int. Ed.* **51**, 4521-4522 (2012). [Obituary]
3. Paul W. Ayers and Ajit Thakkar, "Reduced Density Matrices and Computational Chemistry," *Computational and Theoretical Chemistry* **51**, 4521-4522 (2013). [Prologue]

Journal Articles (Published):

1. Robert C. Morrison and Paul W. Ayers, "Generalized Overlap Amplitudes Using the Extended Koopmans' Theorem for Be"; *J. Chem. Phys.* **103**, 6556-6561 (1995).

2. Paul W. Ayers, Orville W. Day, Jr., and Robert C. Morrison, "Analysis of Density Functionals and Their Density Tails in H_2"; *Int. J. Quantum. Chem.* **69**, 541-550 (1998).
3. Shubin Liu, Paul W. Ayers, and Robert G. Parr, "Alternative Definition of Exchange-Correlation Charge in Density Functional Theory"; *J. Chem. Phys.* **111**, 6197-6203 (1999).
4. Paul W. Ayers and Mel Levy, "Perspective on 'Density Functional Approach to the Frontier-Electron Theory of Chemical Reactivity' by R. G. Parr and W. Yang [J. Am. Chem. Soc. **106**, 4049-4050 (1984)]"; *Theor. Chem. Acc.* **103**, 353-360 (2000).
5. Paul W. Ayers, "Density Per Particle as a Descriptor of Coulomb Systems"; *Proc. Natl. Acad. Sci. USA* **97**, 1959-1964 (2000).
6. Weitao Yang, Yingkai Zhang, and Paul W. Ayers, "Degenerate Ground States and Fractional Number of Electrons in Density and Reduced Density Matrix Functional Theory"; *Phys. Rev. Lett.* **84**, 5172-5175 (2000).
7. Paul W. Ayers and Robert G. Parr, "Variational Principles for Site Selectivity in Chemical Reactivity: The Fukui Function and Chemical Hardness Revisited"; *J. Am. Chem. Soc.* **122**, 2010-2018 (2000).
8. Paul W. Ayers and Robert G. Parr, "A Theoretical Perspective on the Bond Length Rule of Grochala, Albrecht, and Hoffmann"; *J. Phys. Chem. A* **104**, 2211-2220 (2000).
9. Paul W. Ayers, "Atoms in Molecules, an Axiomatic Approach: I. Maximum Transferability"; *J. Chem. Phys.* **113**, 10886-10798 (2000).
10. Paul W. Ayers and Robert G. Parr, "Variational Principles for Describing Chemical Reactions: Reactivity Indices Based on the External Potential"; *J. Am. Chem. Soc.* **123**, 2007-2017 (2001).
11. Paul W. Ayers, "Strategies for Computing Chemical Reactivity Indices"; *Theor. Chem. Acc.* **106**, 271-279 (2001).
12. Paul W. Ayers and Mel Levy, "Sum rules for Exchange and Correlation Potentials"; *J. Chem. Phys.* **115**, 4438-4443 (2001).
13. Paul W. Ayers, Robert C. Morrison, and Ram K. Roy, "Variational Principles for Describing Chemical Reactions: Condensed Reactivity Indices"; *J. Chem. Phys.* **116**, 8731-8744 (2002).
14. Robert G. Parr and Paul W. Ayers, "Representing Potential Energy Surfaces by Expansions in Orthogonal Polynomials. Generalized SPF Potentials"; *J. Phys. Chem. A* (letter) **106**, 5060-5062 (2002).
15. Garnet K-L. Chan, Paul W. Ayers, Edward S. Croot III, "On the Distribution of Eigenvalues of Grand Canonical Density Matrices"; *J. Stat. Phys.* **109**, 289-299 (2002).
16. Paul W. Ayers, Robert G. Parr, and Agnes Nagy, "Local Kinetic Energy and Local Temperature in the Density-Functional Theory of Electronic Structure"; *Int. J of Quantum Chem.* **90**, 309-326 (2002).
17. Paul W. Ayers, and Robert C. Morrison, "Examination of the Monotonic Atomic Density Postulate"; *Acta Chimica et Physica Debrecina* **34-35**, 197-216 (2002). (Gaspar Memorial Issue)
18. Paul W. Ayers, *Julius B. Lucks*, and Robert G. Parr, "Constructing Exact Density Functionals from the Moments of the Electron Density"; *Acta Chimica et Physica Debrecina* **34-35** 223-248 (2002). (Gaspar Memorial Issue)
19. *Qin Wu*, Paul W. Ayers, and Weitao Yang, "Density-Functional Theory Calculations with Correct Long-Range Potentials"; *J. Chem. Phys.* **119**, 2978-2990 (2003).
20. Paul W. Ayers and Robert G. Parr, "Sufficient Conditions for Monotonic Electron Density Decay in Many-Electron Systems"; *Int. J Quantum Chem.* **95**, 877-881 (2003).
21. Paul W. Ayers, "Generalized Christoffel-Darboux Formulae and the Frontier Kohn-Sham Molecular Orbitals"; *Theor. Chem. Acc.* **110**, 267-275 (2003).
22. I. A. Howard, N. H. March, and P. W. Ayers, "Idempotent Density Matrix Derived from a Local Potential V(r) in terms of HOMO and LUMO Properties"; *Chem. Phys. Lett.* (short communication) **385**, 231-232 (2004).
23. Weitao Yang, Paul W. Ayers, and *Qin Wu*, "Potential Functionals: Dual to Density Functionals and Solution to the Upsilon Representability Problem"; *Phys. Rev. Lett.* **92**, 146404 (2004).
24. Frank De Proft, Paul W. Ayers, Kalidas Sen, and Paul Geerlings, "On the Importance of the "Density Per Particle" (Shape Function) in the Density Functional Theory"; *J. Chem. Phys.* **120**, 9969-9973 (2004).
25. Shubin Liu and Paul W. Ayers, "Functional Derivative of the Non-Interacting Kinetic Energy Functional"; *Phys. Rev. A* **70**, 022501 (2004).
26. Bijoy K. Dey, Marek R. Janicki, and Paul W. Ayers, "Hamilton-Jacobi Equation for the Least Action/Least Time Dynamical Path Based on the Fast-Marching Method"; *J. Chem. Phys.* **121**, 6667-6679 (2004).

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259. Paul A. Johnson, Peter A. Limacher, Taewon D. Kim, Michael Richer, Ramon Miranda-Quintana, Farnaz Heidar-Zadeh, Paul W. Ayers, Patrick Bultinck, *Stijn De Baerdemacker*, and Dimtri Van Neck "Strategies for Extending Geminal-Based Wavefunctions: Open Shells and Beyond" *Computational and Theoretical Chemistry* (submitted)
261. R. Miranda-Quintana and P. W. Ayers, "Interpolating Hamiltonians in Chemical Compound Space", *J. Chem. Phys.* (submitted).
262. Ramón Alain Miranda-Quintana, *Marco Martínez González*, *David Hernández-Castillo*, Luis A. Montero-Cabrera, Paul W. Ayers, Christophe Morell, "Conceptual DFT Analysis of the Regioselectivity of 1,3-Dipolar Cycloadditions: Nitrones as a Case Study", *J. Mol. Modelling* (submitted)
263. M. Franco-Pérez, Paul W. Ayers, José L. Gázquez and Alberto Vela,"New Fukui, dual and hyper-dual kernels as bond reactivity descriptors", Theor. Chem. Acc. (submitted).

Journal articles and book chapters from research performed in the Ayers group on which I was not a coauthor: (Group members underlined)

1. Alex D. Bain, Maximo Baron, Steven K Burger, Valdemar J. Kowalewski, and Marina Belin Rodriguez, "Interconversion Study in 1,4-Substituted Six-Membered Cyclohexane-Type Rings. Structure and Dynamics of trans-1,4-Dibromo-1,4-dicyanocyclohexane", *J. Phys. Chem. A*, **115**, 9207–9216 (2011).
2. Peter A. Limacher, Qingxu Xi, and Hans Peter Luthi, "On the effect of electron correlation on the static second hyperpolarizability of π-conjugated oligomer chains", *J. Chem. Phys.* **135**, 014111 (2011).

3. Matthew Chan, *Sergei Manzhos*, Tucker Carrington Jr., Koichi Yamashita, "Parameterized bases for calculating vibrational spectra directly from ab initio data using rectangular collocation," *J. Chem. Th. Comp.* **8**, 2053-2061 (2012).
4. *Meiyan Lou*, Steven K. Burger, *Meghann Gilpin*, *Vivian Gawuga*, Alfredo Capretta and Paul Berti, "Transition State Analysis of Enolpyruvylshikimate 3-Phosphate Synthase (AroA)-Catalyzed EPSP Hydrolysis," *J. Am. Chem. Soc.* **134**, 12947-12957 (2012).
5. *Meiyan Lou*, *Meghann Gilpin*, Steven K. Burger, *Ayesha Malick*, *Vivian Gawuga*, Alfredo Capretta, Paul Berti, "Transition State Analysis of Acid-Catalyzed Hydrolysis of an Enol Ether, Enolpyruvylshikimate 3-Phosphate (EPSP)" *J. Am. Chem. Soc.* **134**, 12958-12969 (2012).
6. Matthew Chan, Koichi Yamashita, Tucker Carrington Jr., and *Sergei Manzhos*, "Toward accurate spectroscopic identification of species at catalytic surfaces: Anharmonic vibrations of formate on AuPt." *MRS Proceedings* 1484 (2012).
7. Ahmed A. K. Mohammed, Peter A. Limacher, Benoît Champagne, "Finding Optimal Finite Field Strengths Allowing for a Maximum of Precision in the Calculation of Polarizabilities and Hyperpolarizabilities" *J. Comp. Chem.* **34**, 1497-1507 (2013).
8. Sergei Manzhos, Matthew Chan, and Tucker Carrington Jr., "Favorable dimensionality scaling of rectangular collocation with adaptable basis functions up to 7 dimensions", *J. Chem. Phys. Communication* **139**, 051101 (2013).
9. Matthew Chan, Tucker Carrington Jr., and Sergei Manzhos, "Anharmonic vibrations of the carboxyl group in acetic acid on TiO_2: implications for adsorption mode assignment in dye-sensitized solar cells" *Phys. Chem. Chem. Phys.* **15**, 10028-10034 (2013).
10. E. C. Varkey, J. Hutter, P. A. Limacher and H. P. Lüthi, "Impact of Donor–Acceptor Functionalization on the Properties of Linearly π-Conjugated Oligomers: Establishing Quantitative Relationships for the Substituent and Substituent Cooperative Effect Based on Quantum Chemical Calculations." *J. Org. Chem.* **78**, 12681-12689 (2013).
11. *Stijn De Baerdemacker*, *Veerle Hellemans*, *Rianne van den Berg*, Jean-Sébastien Caux, Kris Heyde, *Mario Van Raemdonck*, Dimitri Van Neck, Paul A. Johnson, "Probing pairing correlations in Sn isotopes using Richardson-Gaudin integrability" *J. Phys. Conf. Series* **533**, 012058 (2013).
12. Katharina Boguslawski and Markus Reiher, "Chemical Bonding in Open-Shell Transition Metal Complexes" The Chemical Bond: Chemical Bonding Across the Periodic Table. (ed. S. Shaik and G. Frenking) (Wiley, Darmstadt, 2014) pp. 219-252.
13. *M. Mottet,* P. Tecmer, K. Boguslawski, O. Legeza, M. Reiher, "Quantum Entanglement in Carbon-Carbon, Carbon-Phosphorous, and Silicon-Silicon Bonds" *PCCP* **16**, 8872-8880 (2014).
14. Katharina Boguslawski and Pawel Tecmer, "Orbital Entanglement in Quantum Chemistry." *Int. J. Quantum Chem.* **115**, 1289-1295 (2015). [invited perspective]
15. *Sebastian Keller*, Katharina Boguslawski, *Tomasz Janowski*, Markus Reiher and Peter Pulay, "Selection of active spaces for multiconfigurational wavefunctions" *J. Chem. Phys.* **142**, 244104 (2015).
16. Pawel Tecmer, Sung Hong, Katharina Boguslawski, "Dissecting the cation-cation interaction between two uranyl units", Phys. Chem. Chem. Phys. **18**, 18305-18311 (2016).
17. Ramón Alain Miranda-Quintana, "Comments on 'On the non-integer number of particles in molecular system domains: treatment and description'" *Theor. Chem. Acc.* **135**, 1-3 (2016).
18. Ramón Alain Miranda-Quintana, "Condensed-to-atoms hardness kernel from the response of molecular fragment approach" *Chem. Phys. Lett.* **658**, 328-330 (2016).
19. Cercis Morera-Boado, Marco Martínez González, Ramón Alain Miranda-Quintana, Margarita Suárez, Roberto Martínez-Álvarez, Nazario Martín, José M. García de la Vega. "Theoretical study on the mechanism of the thermal retro-cycloaddition of isoxazolinofullerenes", *Journal of Physical Chemistry A*, **120**, 8830-8842 , (2016).
20. Ramón Alain Miranda-Quintana. "Note: The minimum electrophilicity and the hard/soft acid/base principles", *Journal of Chemical Physics*, **146**, 046101 (2017).

21. Ramón Alain Miranda-Quintana, "Density Functional Reactivity Theory" In Conceptual Density Functional Theory (in press).
22. Farnaz Heidar-Zadeh, "Supervised Distance Metric Learning and the Curse of Dimensionality" in Theoretical & Quantum Chemistry at the Dawn of the 21st Century (ed. R. Carbó-Dorca and T. Chakraborty) Apple Academic (in press).
23. Mikhail V. Altaisky, Nadezhda N. Zolnikova, Natalia E. Kaputkina, Victor A. Krylov, Yurii E. Lozovik, Nike Dattani, "Entanglement in a quantum neural network based on quantum dots" *Photonics and Nanostructures* (in press).

2.2 Computer Software

The Ayers group has traditionally been involved in developing new algorithms for (bio)chemical problems. Some of these methods have been released as software (typically through the Ayers group website), including the Fast-Marching Method for finding chemical reaction pathways, *Para-MEAD* for predicting protein pKa, *Para-Freq* for automated parameterization of molecular mechanics force fields, and *GPRI* for computing reactivity indicators from conceptual DFT.

Right now, the group is primarily involved in two large software development projects. All of these research projects were initiated together with researchers from Ghent University, Belgium.

HORTON 2.0.1 (Helpful Open-Source Research Tool for N-fermion systems) In contrast to conventional quantum chemistry software, HORTON is intended primarily as a tool for exploring ideas and developing new methods. To ensure that this is true, we have invested significant time in learning modern software engineering strategies for large open-source projects, and we have occasionally sacrificed some (hopefully not too much) computational performance so that HORTON remains readable and usable even by research communities (e.g., the conceptual density functional theory community) that are uncomfortable with computer programming. This is one reason we decided to write HORTON in the Python language (with selective use of Cython, C++, and Fortran to avoid computational bottlenecks). When cutting-edge computational performance is needed, interfaces to other programs are available. For example, in a recent publication (#209) we used HORTON to generate charges for a molecular dynamics simulation (using the GROMACS package) from the wavefunction generated by another quantum chemistry program (Orca).

HORTON is developed in close collaboration with Toon Verstraelen from the Center for Molecular Modelling (CMM) at Ghent University, Belgium.

Toon Verstraelen, Katharina Boguslawski, Pawel Tecmer, Farnaz Heidar-Zadeh, Matthew Chan, Taewon D. Kim, Yilin Zhao, *Steven Vandenbrande*, Derrick Yang, Cristina E. González-Espinoza, Peter A. Limacher, Diego Berrocal, Ali Malek, Paul W. Ayers HORTON 2.0.0. (2015)
http://theochem.github.com/horton/

CheMPS2 (Density Matrix Renormalization Group software). CheMPS2 is a modern, efficient, parallel, spin- and symmetry-adapted program for optimization matrix product states with the density matrix renormalization group (DMRG) algorithm. Though CheMPS2 can perform general-purpose DMRG calculations, it was designed to be especially suitable for chemical applications. In chemical applications, spin- and symmetry-adaptation can dramatically increase computational efficiency, the virtual dimension of the matrices in the matrix product state is typically greater than 1000, and because not all orbitals are included in the active space, the active space must be optimized (DMRG-SCF). CheMPS2 also has functionality that is specifically interesting for modern quantum chemistry; for example, the seniority pseudosymmetry is implemented, so seniority-zero configuration interaction (also called doubly-occupied CI) calculations can be performed efficiently.

CheMPS2 is primarily developed by Sebastian Wouters, a postdoc working in Dimitri Van Neck's group at the Center for Molecular Modeling (CMM) at Ghent University, Belgium.

S. Wouters, *W. Poelmans*, P.W. Ayers and D. Van Neck, CheMPS2: a free open-source spin-adapted implementation of the density matrix renormalization group for *ab initio* quantum chemistry, *Computer Physics Communications* **185**, 1501-1514 (2014).

Sebastian Wouters, *Ward Poelmans*, *Stijn De Baerdemacker*, Paul W. Ayers, Dimitri Van Neck "CheMPS2: improved DMRG-SCF routine and correlation functions", *Comp. Phys. Commun.* **191**, 235-237 (2015).
https://github.com/SebWouters/CheMPS2

2.3 Invited Talks:

1. Quantum Theory Project Seminar; Univ. of Florida; December 2001 [U.S.A.]
2. Centre Européen de Calcul Atomique et Moléculaire conference: "Exchange Correlation Functionals: Assessment and Prospects"; June 2002 [France]
3. Centre Européen de Calcul Atomique et Moléculaire conference: "Computer modeling of atoms, molecules and materials using approximate functionals of the kinetic energy"; July 2002 [France]
4. 6th Girona Conference on Molecular Similarity; July 2003 [Spain]
5. 10th International Congress on the Applications of Density Functional Theory in Chemistry and Physics; September 2003 [Belgium]
6. Department of Chemistry, North Carolina A&T University; October, 2003 [U.S.A.]
7. Departamento de Química, UAM-Iztapalapa; November 2003 [Mexico]
8. Open Problems and New Directions in Chemical Reactivity and Density-Functional Theory; November 2003) [Mexico]
9. Department of Chemistry, East Carolina University; November 2003 [U.S.A.]
10. Singapore International Chemistry Conference; "Frontiers in Physical and Analytical Chemistry"; December 2003 [Singapore]
11. Department of Chemistry; University of Western Ontario, January, 2004. [Canada]
12. Frontiers of Quantum Chemical Modelling and Simulation, CSC Conference; May 2004. [Canada]
13. 15th Canadian Symposium on Theoretical Chemistry; July 2004. [Canada]
14. Laboratoire de Chimie Theorique; Centre Nationale de la Reserche Scientifique; December 2004. [France]
15. Department of Chemistry; Vrije Universiteit Brussel; December 2004. [co-organized by Association of Belgian Quantum Chemists] [Belgium]
16. Department of Mathematics; McMaster University; January 2005. [Canada]
17. Department of Chemistry; The University of North Carolina at Chapel Hill; April 2005. [U.S.A.]
18. Department of Chemistry; East Carolina University; April 2005. [U.S.A.]
19. Departments of Chemistry/Physics; Cornell University; Electronic Structure Seminar; May, 2005. [U.S.A.]
20. Canadian Society for Chemistry 2005 Annual Meeting ("Trends in Theoretical and Computational Chemistry"); May, 2005. [Canada]
21. 5th Congress of the International Society for Theoretical Chemical Physics; July, 2005. [U.S.A.]
22. Department of Chemistry; Kansas State University; August, 2005. [U.S.A.]
23. Electron densities and density functionals (part of the International Conference of Computational Methods in Sciences and Engineering); October 2005. [Greece]
24. Reactivity descriptors: Conceptual and computational developments (part of the International Conference of Computational Methods in Sciences and Engineering); October 2005. [Greece]
25. Institute of Theoretical Physics; University of Ghent; November, 2005 [co-organized by Association of Belgian Quantum Chemists]. [Belgium]
26. Pacifichem (December 2005) [U.S.A.]
27. 231st National Meeting of the American Chemical Society "Frontier Applications and Developments of Density Functional Theory" (March 2006) [U.S.A.]
28. Solvay Congress on "Theoretical Aspects of Chemical Reactivity" (April 2006) [Belgium]
29. Canadian Society of Chemistry Conference 2006 Annual Meeting ("Ab initio Methods: Orbital and Plane Wave Methods") (May 2006) [Canada]
30. 7th Girona Conference on The Nature of the Chemical Bond; Girona, Spain (July 2006) [Spain]
31. 6th Canadian Computational Chemistry Conference (July 2006) [Canada]
32. Faraday Discussion 135: Chemical Concepts from Quantum Mechanics (September 2006) [U.K.]
33. Workshop on Mathematical Methods for *Ab Initio* Quantum Chemistry; University of Nice, France (October 2006) [France]
34. Oberwolfach Workshop on Mathematical and Numerical Aspects of Quantum Chemistry Problems (October 2006) [Germany]
35. Symposium on concepts in density-functional theory; Grenoble, France (October 2006). [France]

36. Minisimposio en Química Teórica Y Computacional (January, 2007). [Chile]
37. Department of Physics; University of Chile (January, 2007) [Chile]
38. Department of Chemistry; University of Andres Bello (January, 2007) [Chile]
39. 47th Sanibel Symposium [plenary lecture] (February 2007) [U.S.A.]
40. Theoretical Chemistry Group at Duke University (March, 2007) [U.S.A.]
41. Computational Biology Group at National Institutes of Environment Health Sciences (March, 2007) [U.S.A.]
42. Department of Chemistry; University of Waterloo (May 2007) [Canada]
43. Symposium on Biocomputational Chemistry, Canadian Chemistry Society Conference (May 2007) [Canada]
44. Symposium on Computational Chemistry in Chemical Education, Canadian Chemistry Society Conference (May 2007) [Canada]
45. Symposium on concepts in density-functional theory (June 2007) [Belgium]
46. Institute of Mathematics and its Applications (IMA) Summer Program (August 2007) [U.S.A.]
47. DFT2007; 12th International Conference on the Theory and Applications of Density Functional Theory (August 2007) [The Netherlands]
48. Department of Chemistry, ETH-Zurich (co-hosted by ETH, Univ. Zurich, and IBM-Zurich) (October 2007) [Switzerland]
49. Department of Chemistry, Univ. of Geneva (October 2007) [Switzerland]
50. Waterloo Chemical Physics Conference (November 2007) [Canada]
51. Department of Physics; University of Chile (January, 2008) [Chile]
52. Department of Chemistry; University of Andres Bello (January, 2008) [Chile]
53. Department of Chemistry; Brock University (February, 2008) [Canada]
54. Centre for Research in Molecular Modeling Symposium (April 2008) [Canada]
55. Workshop on Range Separation Hybrids in Density-Functional Theory (May 2008) [France]
56. Center for Molecular Modeling at Univ. of Ghent (May 2008) [Belgium]
57. Department of Chemistry; Hong Kong University of Science and Technology (June 2008) [Hong Kong]
58. Department of Physics and Materials Science; City University of Hong Kong (June 2008) [Hong Kong]
59. Department of Chemistry; South China Normal University (June 2008) [China]
60. Department of Chemistry; South China University of Technology (June 2008) [China]
61. Department of Chemistry; Hunan Normal University (June 2008) [China]
62. 2008 Symposium on Computational Chemistry and HPC Applications (June 2008) [China]
63. Shanghai Institute of Materia Medica (July 2008) [China]
64. 8th Girona Conference on Aromaticity (July 2008) [Spain]
65. Symposium on Density Functional Theory dedicated to Prof. José Luis Gázquez Mateos on the occasion of his 60th birthday (October 2008) [Mexico]
66. Facultad de Quimica; Universidad de Guanajuato; Lecture Series with 4 talks (October 2008) [Mexico]
67. Department of Chemistry; Beijing University; Lecture Series with 4 talks (November 2008) [China]
68. Department of Chemistry,Tsinghua University (November 2008) [China]
69. Dept. of Chemistry, Beijing Normal University (November 2008) [China]
70. Chinese Academy of Sciences, Shanghai Institute for Organic Chemistry; "overview" of computational chemistry" (November 2008) [China]
71. Laboratoire de Chimie Theorique; Centre Nationale de la Reserche Scientifique; (Dec. 2008) [France]
72. Department of Chemistry; University of Andres Bello (January, 2009) [Chile]
73. Department of Chemistry, York University (February 2009) [Canada]
74. Department of Chemistry, Queen's University (February 2009) [Canada]
75. 2009 Molecular Informatics and Bioinformatics Symposium (March 2009) [Hungary]
76. Girona Workshop on Theoretical Chemistry (July 2009) [Spain]
77. Seventh Canadian Computational Chemistry Conference (July 2009) [Canada]
78. Fields Institute Workshop on Quantum Marginals and Density Matrices (July 2009) [Canada]
79. 33rd International Workshop on Condensed Matter Theories (August 2009) [Ecuador]
80. Department of Chemistry, Wayne State University (November, 2009) [U.S.A.]

81. Symposium "Of Molecules and Materials; A Survey of Recent Concepts" at Indian Institute for Scientific Education and Research (December, 2009) [India]
82. Symposium in the Theoretical Sciences, IIT-Kharagpur (December, 2009) [India]
83. Center for Theoretical Science, IIT-Kharagpur (January 2010) [India]
84. Indian Association for the Cultivation of Science, (January 2010) [India]
85. Department of Chemistry, Calcutta University, (January 2010) [India]
86. Symposium on Quantum Chemistry, Pontificia Universidad Católica de Chile (January 2010)[Chile]
87. Sanibel Symposium (February 2010) [U.S.A.]
88. Department of Chemistry, Duke University (theoretical chemistry seminar) [U.S.A.]
89. Department of Chemistry, New York University (April 2010) [U.S.A.]
90. Quantum Theory Project, University of Florida; 3 talks (April 2010) [U.S.A.]
91. Brookhaven National Laboratory (April 2010) [U.S.A.]
92. FANTOM Study Week, Ghent University; Lecture Series with 2 Talks (May 2010) [Belgium]
93. Canadian Society for Chemistry Conference (May 2010) [Canada]
94. 20th Birthday Conference for the Electron Localization Function (June 2010) [France]
95. Gordon Conference, "Electron Densities and Chemical Bonding" (July 2010) [opening lecture] [U.S.A.]
96. National Science Foundation Workshop on Software Infrastructure for Scientific Innovation (July 2010) [opening "perspective" lecture] [U.S.A.]
97. 9th Girona Seminar, "Electron Density, Density Matrices, and Density-Functional Theory" (July 2010) [Spain]
98. "Challenges in Density Functional Theory" at American Chemical Society National Meeting (August 2010) [U.S.A.]
99. Girona Workshop on Theoretical Chemistry (October 2010) [Spain]
100. Department of Chemistry; Purdue University (November 2010) [U.S.A.]
101. Department of Chemistry; University of Ottawa (December 2010) [Canada]
102. Department of Chemistry; Dalhousie University (December 2010) [Canada]
103. Pacifichem (December 2010) [U.S.A.]
104. Pacifichem (December 2010) [U.S.A.]
105. Pacifichem (December 2010) [U.S.A.]
106. Universidad de Chile; Dept. of Physics. (January 2011) [Chile]
107. Quantum Theory Project; Univ. of Florida (January 2011) [U.S.A.]
108. Dept. of Chemistry; Univ. of Florida (January 2011) [U.S.A.]
109. Dept. of Chemistry, Laval Univeristy (February 2011) [Canada]
110. Dept. of Chemistry, Tulane University (March 2011) [U.S.A.]
111. First Annual DFT-Day (April 2011) [Chile]
112. Physical Frameworks for Sampling Chemical Compounds Space; Institute for Pure and Applied Mathematics (May 2011) [U.S.A.]
113. Canadian Society for Chemistry (June 2011) [award lecture; Canada]
114. European Seminar on Computational Methods in Quantum Chemistry (June 2011) [Norway]
115. 9th Conference of the World Association of Theoretically Oriented Chemists (July 2011) [Spain]
116. Telluride Meeting on New Frontiers in Electron Correlation (July 2011) [U.S.A.]
117. 47th Symposium for Theoretical Chemistry (August, 2011) [Switzerland]
118. 242nd American Chemical Society National Meeting (August 2011) [U.S.A.]
119. 242nd American Chemical Society National Meeting (August 2011) [U.S.A.]
120. 7th Congress of the International Society for Theoretical Chemical Physics (August 2011) [Japan]
121. Prague Workshop on Theoretical Chemistry (September 2011) [Czech Republic]
122. Workshop on Maximum Probability Domains (November 2011) [France]
123. Summer Talks in Santiago (STS); Symposium on Quantum Chemistry, Pontificia Universidad Católica de Chile (January 2012) [Chile]
124. Satellite Symposium of STS; "Topics in DFT and Chemical Reactivity" (January 2012) [Chile]
125. Universidad de Chile; Dept. of Physics. (January 2012) [Chile]

126. 2nd Annual DFT Day (January 2012) [Chile]
127. Acenet Lecturer; Department of Chemistry, Univ. of New Brunswick (February 2012) [Canada]
128. Acenet Lecturer; Department of Chemistry, Dalhousie University (February 2012) [Canada]
129. Acenet Lecturer; Department of Chemistry, Cape Breton University (February 2012) [Canada]
130. Acenet Lecturer; Department of Chemistry, Memorial University of Newfoundland (March 2012) [Canada]
131. 243rd National Meeting of the American Chemical Society (March 2012) [U.S.A.]
132. Challenges in Density Matrix and Density Functional Theory (April 2012) [plenary, Belgium]
133. Conceptual DFT & QSAR Worshop (April 2012) [Belgium]
134. Kathmandu 2012 Workshop on Theoretical Chemistry (April 2012) [Nepal]
135. Theoretical Chemistry Seminar; Duke University (May 2012) [U.S.A.]
136. Inaugural Changsha Workshop on Theoretical and Computational Chemistry (June 2012) [China]
137. School of Chemistry, Hunan Normal University (June 2012) [China]
138. Institute for Organic Chemistry, Chinese Academy of Sciences (June 2012) [China]
139. 2nd Workshop on Sparse Grids and Applications (July 2012) [Germany]
140. Sagamore XVII Workshop (July 2012) [Japan]
141. 25th Canadian Symposium on Theoretical and Computational Chemistry (July 2012) [Canada]
142. 2nd International Symposium on Electron Momentum Spectroscopy (August 2012) [Belgium]
143. Dept. of Chemistry, Univ. of Florida; 2 talks (September 2012) [U.S.A.]
144. Workshop on New Methods in Electronic Structure Theory (October 2012) [Belgium]
145. 7th Singapore International Chemistry Conference (December 2012) [Singapore]
146. Indian Theoretical Chemistry Symposium (TCS) (December 2012) [India]
147. 3rd Annual DFT Days (January 2013) [Chile]
148. Department of Chemistry, Dalhousie University (February 2013) [Canada]
149. 53rd Sanibel Symposium (February 2013) [U.S.A.]
150. Understanding, Discovering, and Enlighting Chemistry, An International Symposium on Theoretical & Computational Chemistry (March 2013) [Chile]
151. Department of Physics; Universidad de Chile (March 2013) [Chile]
152. 245th American Chemical Society National Meeting (April 2013) [U.S.A.]
153. Theoretical Chemistry Seminar, Duke University (April 2013) [U.S.A.]
154. Canadian Society for Chemistry (May 2013) [Canada]
155. 7th Molecular Quantum Mechanics Meeting (June 2013) [Switzerland]
156. Very Accurate and Large Computations and Applications (June 2013) [Norway]
157. 2nd Changsha Workshop on Theoretical and Computational Chemistry (June 2013) [China]
158. 8th International Congress of the International Society of Theoretical Chemical Physics (August 2013) [Hungary]
159. Laboratory of Theoretical Chemistry, Eötvös University (August 2013) [Hungary]
160. Theoretical Group Seminar, Dept. of Chemistry, Rice University (August 2013) [U.S.A.]
161. Current Trends in Theoretical Chemistry 2013 (September 2013) [India]
162. Advances in Quantum Chemical Topology (October 2013) [Mexico]
163. International Workshop on Computational Science and Engineering (October 2013) [Taiwan]
164. Annual Symposium on Drug Design; 11th 11th Annual Congress of International Drug Discovery Science and Technology (November 2013) [China]
165. International Workshop on High Dimensional Data Approximation (November 2013) [China]
166. Symposium in Honor of Norman H. March (November 2013) [Belgium]
167. Canada Days Workshop (November 2013) [Belgium]
168. McMaster Computational Sciences Seminar (February 2014) [Canada]
169. Theoretical Chemical Physics Group; University of Toronto (March 2014) [Canada]
170. March Meeting of the American Physical Society (March 2014) [U.S.A.]
171. Departments of Chemistry and Physics, Universidad de Antioquia (April 2014) [Colombia] (lecture series with 3 talks)

172. V Colombian Congress in Theoretical and Computational Chemistry (April, 2014) [Colombia] (lectures series with 3 talks)
173. Low-Scaling and Unconventional Electronic Structure Theory Methods; Telluride Scientific Research Conference. (June 2013) [U.S.A.]
174. 3rd Changsha Workshop on Theoretical and Computational Chemistry (June 2014) [China]
175. Steacie Prize Lecture; McMaster University (June 2014) [Canada]
176. International Conference on Chemical Bonding (July 2014) [U.S.A.]
177. 2nd International Conference on Computational Science and Engineering [Vietnam]
178. Current Topics in Theoretical Chemistry (August 2014) [Vietnam]
179. International Conference on Theoretical and High Performance Computational Chemistry (September 2014) [China]
180. Beijing University of Chemical Technology (September 2014) [China]
181. Computational Challenges in Nuclear and Many-Body Physics (Nordita) (September 2014) [Sweden]
182. World Association of Theoretically-Oriented Chemists Conference (October 2014) [Chile] [plenary award lecture]
183. WATOC 2014 Satellite: Large Condensed and Biological Systems (October 2014) [Chile]
184. Origins Colloquium, McMaster University (October 2014) [Canada].
185. Quantum Systems in Chemistry and Physics XIX (November 2014) [Taiwan] [plenary lecture]
186. Department of Chemistry, University of Western Ontario (December 2014) [Canada]
187. Department of General Chemistry; Vrije Universiteit Brussel (December 2014) [Belgium]
188. Institut de Calcul et de la Simulation, Sorbonne Universites (December 2014) [Paris]
189. Fundamental Aspects of DFT Workshop (January 2014) [Norway]
190. Department of Physical Chemistry; ETH-Zürich (Janauary 2015) [Switzerland] (lecture series with 2 talks)
191. Department of Physical Chemistry; University of Basel (January 2015) [Switzerland]
192. Initiative for the Theoretical Sciences Seminar; Graduate Center of the City University of New York (February 2015) [U.S.A.]
193. 55th Sanibel Symposium (February 2015) [U.S.A.]
194. International Workshop on New Frontier of Numerical Methods for Many-Body Correlations: Methodologies and Algorithms for Fermion Many-Body Problems (February 2015) [Japan]
195. Machine Learning for Many Particle Systems; Institute for Pure And Applied Mathematics at the University of California, Los Angeles (UCLA) (February 2015) [U.S.A.]
196. Centre for Molecular Simulation, University of Calgary (March 2015) [Canada]
197. Division of Materials Science; Nanyang Technological University (March 2015) [Singapore]
198. Department of Physics, University of Buenos Aires (March 2015) [Argentina]
199. Advances in Electronic Structure Theory (April 2015) [France]
200. Recent Advances in Electronic Structure Theory (June 2015) [China]
201. International Congress of Quantum Chemistry (June 2015) [China]
202. Chemical Bonds at the 21st Century (June 2015) [China]
203. Telluride Workshop on New Frontiers in Electron Correlation (July 2015) [U.S.A.]
204. 16th International Conference on Density Functional Theory and its Applications [Hungary] (August 2015)
205. M4 Meeting II (Meeting on Methods for Modeling Molecules and Materials) (September 2015) [Canada]
206. Theoretical Chemistry Seminar; Duke University (September, 2015) [U.S.A.]
207. Workshop on Maximum Probability Domains (October 2015) [Belgium]
208. Kapuy Lecture, Eotvos Lorand University (October 2015) [Hungary]
209. Center for Multiscale Theory and Computation, Univ. Münster (November 2015) [Germany]
210. Institute for Organic Chemistry, Universitat Münster (November 2015) [Germany]
211. Virtual Winter School on Computational Chemistry (Feb. 2016) [online]
212. Kobe Workshop on Materials Design on Strongly-Correlated Electrons in Molecules and Materials, RIKEN Advanced Institute for Computational Sciences (K Computer) (February 2016) [Japan]
213. Workshop on Computation of Quantum Systems in Cold-matter Physics and Chemistry; Fields Institute

(March 2016) [Canada]

214. Symposium on New Generation Quantum Theory -Particle Physics, Cosmology, and Chemistry; Univ. of Kyoto (March 2016) [Japan]
215. Solvay Workshop on "Solvay Workshop on "Conceptual Quantum Chemistry: Present Aspects and Challenges for the Future" (April, 2016) [Belgium]
216. CECAM Workshop on "Exploring Chemical Space with Machine Learning and Quantum Mechanics" (June, 2016) [Switzerland]
217. Canadian Society for Chemistry Conference (June, 2016) [Canada]
218. Department of Chemistry; Lipscomb University (June, 2016) [USA]
219. Changsha Workshop on Theoretical Chemistry (June, 2016) [China]
220. Quantum Systems in Chemistry and Physics (July, 2016) [Canada]
221. Canadian Theoretical and Computational Chemistry Conference (July, 2016) [Canada]
222. International Symposium on Theoretical Chemical Physics (July, 2016) [USA]
223. Theory and Applications of Computational Chemistry (August 2016) [USA]
224. Current Trends in Theoretical Chemistry (September 2016) [Poland]
225. Theoretical Chemistry Group Seminar, Duke University (September, 2016) [USA]
226. Current Topics in Theoretical Chemistry School (September 2016) [Peru]
227. Current Topics in Theoretical Chemistry (September 2016) [Peru]
228. EMN Meeting on Density Functional Theory (October 2016) [USA]
229. Ghent Theoretical Chemistry Workshop on Geminals Methods (October 2016) [Belgium]
230. International Symposium of Computational Organometallic Catalysis 2016 (October 2016) [China]
231. Dept. of Chemistry, Duke University (October, 2016) [USA]
232. Perspectives on Catalysis and Energy (November 2016) [Chile]
233. XV Reunión Mexicana de Fisicoquímica Teórica (Nov. 2016) [Mexico]
234. Ghent Theoretical Chemistry Workshop on Maximum Probability Domains (December 2016) [Belgium]
235. Dept. of Chemical & Materials Engineering; National University of Singapore (Jan. 2017) [Singapore]
236. Dept. of Chemistry; University of North Texas (Davidson Lecture) [2 lectures] (Feb. 2017) [U.S.A.]
237. Dept. of Chemistry; Univ. of Buffalo (Foster Colloquium) (Feb. 2017) [U.S.A.]
238. HORTON/ChemTools Workshop (Univ. de Chile) (March 2017) [Chile]
239. DFT-Days; (Univ. de Chile) (March 2017) [Chile]

2.4 Contributed Talks:

233rd National Meeting of the American Chemical Society (March 2007) [U.S.A.]
Canadian Society for Chemistry (June 2011) [Canada]
247th National Meeting of the American Chemical Society (March 2014) [U.S.A.]

2.5 Posters:

Paul W. Ayers; Analysis of Density Functionals and Their Density Tails (Symposium on Density Functional Theory and Applications: A Satellite Symposium of the 9th International Congress on Quantum Chemistry; June 1997) [U.S.A.]
Paul W. Ayers; Density Generated Basis Functions (Pitzer Symposium; Jan. 2000) [U.S.A.]
Paul W. Ayers; Beyond Basis Sets: Cubature Methods for Molecular Quantum Mechanics (Sanibel Symposium; Feb. 2002) [U.S.A.]
Paul W. Ayers; Generalizations of the Hohenberg-Kohn Theorem (10th International Congress on the Applications of Density Functional Theory in Chemistry and Physics; September 2003) [Belgium]

2.6 Public Lectures:

Lecture on "Science in Society" at Highland Secondary School in Dundas (May, 2003).
Steacie Prize Lecture; McMaster University (June, 2015)

2.7 Invited Lecture Series

IBM-Zürich Lecture Series (Switzerland, 2007)
Acenet Lecture Series (Atlantic Canada, 2012)
Ede Kapuy Lecture (Hungary, 2015)
Davidson Lecture (U.S.A., 2017)

Foster Colloquium (U.S.A., 2017)

2.8 Talks/Posters by Supervisees:

1. Graduate Student Symposium at the University of Buffalo; Univ. of Buffalo, United States (James Anderson; May 2005) [poster] [U.S.A.]
2. Graduate Student Symposium at the University of Buffalo; Univ. of Buffalo, United States (Juan Rodriguez; May 2005) [poster] [U.S.A.]
3. Recent Developments in Electronic Structure; Cornell Univ., United States (James Anderson; June 2005) [poster] [U.S.A.]
4. Simulation of Rare Events, The Reaction-Path Problem in Complex Systems; CECAM, France (Bijoy Dey; June 2005) [poster] [France]
5. Nanoscience at the Interface of Chemistry and Biology, Cancun, Mexico (Juan Rodriguez; August 2005) [talk] [Mexico]
6. Graduate Student Symposium at the University of Buffalo; Univ. of Buffalo, United States (James Anderson; May 2006) [talk] [U.S.A.]
7. EMBO Course/Conference on "Proteins: Structure, Dynamics, and Energetics" at the Shanghai Institute for Biological Sciences; Shanghai, China. (Annie Liu; May 2006) [poster]. [China]
8. 6th European Conference on Computational Chemistry (Juan Rodriguez, August 2006) [poster]. [Slovakia]
9. Graduate School of Physics; Instituto Politecnico Nacional de Mexico (IPN) (Juan Rodriguez, December 2006) [invited talk] [Mexico]
10. 234th National Meeting of the American Chemical Society. (James Anderson, August 2007) [talk] [U.S.A.]
11. 234th National Meeting of the American Chemical Society. (James Anderson, August 2007) [poster] [U.S.A.]
12. 234th National Meeting of the American Chemical Society. (Juan Rodriguez, August 2007) [poster] [U.S.A.]
13. 235th National Meeting of the American Chemical Society. (Ivan Vinogradov, April 2008) [poster] [U.S.A.]
14. Women in Science and Engineering Conference (Annie Liu, April 2008) [talk] [Canada]
15. Canadian Chemistry Society Conference (Annie Liu, May 2008) [talk] [Canada]
16. Canadian Chemistry Society Conference (James Anderson, May 2008) [talk] [Canada]
17. Canadian Chemistry Society Conference (Ivan Vinogradov, May 2008) [talk] [Canada]
18. Canadian Chemistry Society Conference (Rogelio Cuevas, May 2008) [talk] [Canada]
19. Odyssey 2008, Mathematical and Computational Aspects of Molecular Electronic Structure Calculations (James Anderson, June 2008) [talk] [Canada]
20. Odyssey 2008, Mathematical and Computational Aspects of Molecular Electronic Structure Calculations (Rogelio Cuevas, June 2008) [talk] [Canada]
21. NSERC-USRA Undergraduate Student Poster Competition (Sandra Rabi, January 2009) [poster] [Canada]
22. Universidad de Guanajuato (Carlos Cardenas, January 2009) [invited talk] [Mexico]
23. Dept. of Physics; Higher School of Physics and Mathematics of the National Polytechnic Institute (Rogelio Cuevas, February 2009) [invited talk] [Mexico]
24. Southern Ontario Undergraduate Chemistry Conference (Sandra Rabi; March 2009) [talk] [Canada]
25. Women in Science and Engineering Conference (Nataly Rabi; March 2009) [poster] [Canada]
26. Center for Research in Molecular Modeling (Debajit Chakraborty; May 2009) [poster] [Canada]
27. New York Graduate Student Symposium at the Univ. of Buffalo (James Anderson; May 2009) [talk] [U.S.A.]
28. New York Graduate Student Symposium at the Univ. of Buffalo (Rogelio Cuevas; May 2009) [talk] [U.S.A.]
29. Canadian Society for Chemistry Conference (Sandra Rabi, June 2009) [poster] [Canada]
30. Canadian Society for Chemistry Conference (Carlos Cardenas, June 2009) [poster] [Canada]
31. Canadian Society for Chemistry Conference (Nataly Rabi, June 2009) [poster] [Canada]
32. Canadian Society for Chemistry Conference (Debajit Chakraborty, June 2009) [poster] [Canada]
33. Canadian Society for Chemistry Conference (Rogelio Cuevas, June 2009) [invited talk] [Canada]
34. Canadian Society for Chemistry Conference (James Anderson, June 2009) [invited talk] [Canada]
35. Canadian Society for Chemistry Conference (Steven Burger, June 2009) [talk] [Canada]
36. Canadian Society for Chemistry Conference (Eleonora Echegaray, June 2009) [talk] [Canada]
37. Canadian Society for Chemistry Conference (Paul Johnson, June 2009) [talk] [Canada]
38. Fields Institute Workshop on Quantum Marginals and Density Matrices (Paul Johnson, July 2009) [Canada]
39. Fields Institute Workshop on Quantum Marginals and Density Matrices (Carlos Cardenas, July 2009) [Canada]
40. Fields Institute Workshop on Quantum Marginals and Density Matrices (Rogelio Cuevas, July 2009) [Canada]
41. Fields Institute Workshop on Quantum Marginals and Density Matrices (Pavel Kulikov, July 2009) [Canada]

42. Fields Institute Workshop on Quantum Marginals and Density Matrices (James Anderson, July 2009) [Canada]
43. Seventh Canadian Computational Chemistry Conference (Rogelio Cuevas, July 2009) [poster] [Canada]
44. Seventh Canadian Computational Chemistry Conference (Ivan Vinogradov, July 2009) [poster] [Canada]
45. Seventh Canadian Computational Chemistry Conference (Carlos Cardenas, July 2009) [poster] [Canada]
46. Seventh Canadian Computational Chemistry Conference (Eleonora Echegaray, July 2009) [poster] [Canada]
47. DFT2009; 13th International Conference on the Theory and Applications of Density Functional Theory (Carlos Cardenas, August 2009) [poster] [France]
48. Theoretical Chemistry Group, Beijing University (James Anderson, October 2009) [invited talk] [China]
49. Department of Chemistry; Vrije Universiteit Brussels (Carlos Cardenas, Oct. 2009) [invited talk] [Belgium]
50. Departments of Chem. and Phys.; UAM-Iztapalapa (Carlos Cardenas, Nov. 2009) [invited talk] [Mexico]
51. Waterloo Chemical Physics Conference (Paul Johnson, November 2009) [poster] [Canada]
52. Waterloo Chemical Physics Conference (Debajit Chakraborty, November 2009) [poster] [Canada]
53. Waterloo Chemical Physics Conference (Helen Van Aggelen, November 2009) [poster] [Canada]
54. Waterloo Chemical Physics Conference (Steven Burger, November 2009) [talk] [Canada]
55. Waterloo Chemical Physics Conference (Rogelio Cuevas, November 2009) [talk] [Canada]
56. 41st Inorganic Discussion Weekend (Paul Johnson, November 2009) [talk] [Canada]
57. Undergraduate Student Research Award Poster Session (Paul Johnson, November 2009) [poster] [Canada]
58. Department of Chemistry, Univ. Andres Bello (Carlos Cardenas, December 2009) [invited talk] [Chile]
59. American Chemical Society National Meeting (Rogelio Cuevas, March 2010) [poster] [U.S.A.]
60. American Chemical Society National Meeting (Ivan Vinogradov, March 2010) [poster] [U.S.A.]
61. Department of Chemistry, Wayne State University (Steven Burger, April 2010) [invited talk] [Canada]
62. Women in Science and Engineering Conference (Sandra Rabi; March 2010) [talk] [Canada]
63. Graduate Student Symposium at the University of Buffalo; Univ. of Buffalo, United States (James Anderson; May 2010) [talk] [U.S.A.]
64. Graduate Student Symposium at the University of Buffalo; Univ. of Buffalo, United States (Paul Johnson; May 2010) [talk] [U.S.A.]
65. Canadian Society for Chemistry Conference (Steven Burger, June 2010) [talk] [Canada]
66. Canadian Society for Chemistry Conference (Nataly Rabi, June 2010) [poster] [Canada]
67. Canadian Society for Chemistry Conference (Rogelio Cuevas, June 2010) [poster] [Canada]
68. Canadian Society for Chemistry Conference (Rogelio Cuevas, June 2010) [poster] [Canada]
69. Canadian Society for Chemistry Conference (Paul Johnson, June 2010) [poster] [Canada]
70. Canadian Society for Chemistry Conference (Paul Johnson, June 2010) [poster] [Canada]
71. Canadian Society for Chemistry Conference (Eleonora Echegaray, June 2010) [poster] [Canada]
72. Canadian Society for Chemistry Conference (Debajit Chakraborty, June 2010) [poster] [Canada]
73. Canadian Society for Chemistry Conference (Ahmed Mohammed, June 2010) [poster] [Canada]
74. Canadian Society for Chemistry Conference (James Anderson, June 2010) [poster] [Canada]
75. Gordon Research Conference (Eleonora Echegary, July 2010) [poster] [U.S.A.]
76. International Symposium on Molecular Dynamics and Reactivity (Eleonora Echegary, July 2010) [invited talk] [Canada]
77. International Symposium on Molecular Dynamics and Reactivity (Steven Burger, July 2010) [invited talk] [Canada]
78. International Symposium on Molecular Dynamics and Reactivity (Annie Liu, July 2010) [invited talk] [Canada]
79. Waterloo Chemical Physics Conference (Steven Burger, November 2010) [talk] [Canada]
80. Waterloo Chemical Physics Conference (Debajit Chakraborty, November 2010) [poster] [Canada]
81. Waterloo Chemical Physics Conference (Farnaz Heidarzadeh, November 2010) [poster] [Canada]
82. Waterloo Chemical Physics Conference (Sandra Rabi, November 2010) [poster] [Canada]
83. Waterloo Chemical Physics Conference (Rogelio Cuevas, November 2010) [poster] [Canada]
84. Waterloo Chemical Physics Conference (Paul Johnson, November 2010) [poster] [Canada]
85. Current Research in Science and Technology (Farnaz Heidarzadeh, March 2011) [talk] [Canada]
86. Current Research in Science and Technology (Sandra Rabi, March 2011) [talk] [Canada]
87. 2nd International Symposium on Molecular Dynamics and Reactivity (Steven Burger, May 2011) [Invited Talk] [Canada]
88. 2nd International Symposium on Molecular Dynamics and Reactivity (Annie Liu, May 2011) [Invited Talk] [Canada]

89. 2nd International Symposium on Molecular Dynamics and Reactivity (Sandra Rabi, May 2011) [Invited Talk] [Canada]
90. 2nd International Symposium on Molecular Dynamics and Reactivity (Debajit Chakraborty, May 2011) [Invited Talk] [Canada]
91. 2nd International Symposium on Molecular Dynamics and Reactivity (Rogelio Cuevas, May 2011) [Invited Talk] [Canada]
92. 2nd International Symposium on Molecular Dynamics and Reactivity (Paul Johnson, May 2011) [Invited Talk] [Canada]
93. Canadian Society for Chemistry Conference (Sandra Rabi, June 2011) [talk] [Canada]
94. Canadian Society for Chemistry Conference (Sandra Rabi, June 2011) [talk] [Canada]
95. Canadian Society for Chemistry Conference (Debajit Chakraborty, June 2011) [poster] [Canada]
96. Canadian Society for Chemistry Conference (Rogelio Cuevas, June 2011) [talk] [Canada]
97. Canadian Society for Chemistry Conference (Rogelio Cuevas, June 2011) [talk] [Canada]
98. 3rd International Symposium on Molecular Dynamics and Reactivity (Steven Burger, June 2011) [Invited Talk] [Canada]
99. 3rd International Symposium on Molecular Dynamics and Reactivity (Annie Liu, June 2011) [Invited Talk] [Canada]
100. 3rd International Symposium on Molecular Dynamics and Reactivity (Sandra Rabi, June 2011) [Invited Talk] [Canada]
101. 3rd International Symposium on Molecular Dynamics and Reactivity (Farnaz Heidarzadeh, June 2011) [Invited Talk] [Canada]
102. International Conference on Applied Mathematics, Modeling, and Computational Science (Steven Burger, July 2011) [invited talk] [Canada]
103. International Conference on Applied Mathematics, Modeling, and Computational Science (Rogelio Cuevas, July 2011) [talk] [Canada]
104. International Conference on Applied Mathematics, Modeling, and Computational Science (Rogelio Cuevas, July 2011) [talk] [Canada]
105. 4th International Symposium on Molecular Dynamics and Reactivity (Debajit Chakraborty, July 2011) [Invited Talk] [Canada]
106. 4th International Symposium on Molecular Dynamics and Reactivity (Rogelio Cuevas, July 2011) [Invited Talk] [Canada]
107. 4th International Symposium on Molecular Dynamics and Reactivity (Farnaz Heidarzadeh, July 2011) [Invited Talk] [Canada]
108. 4th International Symposium on Molecular Dynamics and Reactivity (Peter Limacher, July 2011) [Invited Talk] [Canada]
109. 4th International Symposium on Molecular Dynamics and Reactivity (Helen Van Aggelen, July 2011) [Invited Talk] [Canada]
110. 14th International Conference on the Theory and Applications of Density Functional Theory (Paul Johnson, August 2011) [talk] [Greece]
111. 7th Congress of the International Society for Theoretical Chemical Physics (Peter Limacher, August 2011) [poster] [Japan]
112. Centrum Voor Moleculaire Modeling, Universiteit Gent (Paul Johnson, Oct. 2011) [Invited Talk] [Belgium]
113. Department of Chemistry; Mount St. Vincent Univ. (Farnaz Heidarzadeh, Oct. 2011) [invited talk] [Canada]
114. Laboratoire de Chimie Theorique, Centre National de la Recherche Scientifique (Paul Johnson, Oct. 2011) [Invited Talk] [France]
115. Theoretical Chemistry Research Group, ETH Zurich (Paul Johnson, Nov. 2011) [Invited Talk] [Switzerland]
116. Waterloo Chemical Physics Conference (Steven Burger, November 2011) [poster] [Canada]
117. Waterloo Chemical Physics Conference (Santa Rabi, November 2011) [poster] [Canada]
118. Waterloo Chemical Physics Conference (Christopher Haddad, November 2011) [poster] [Canada]
119. Waterloo Chemical Physics Conference (Sandra Rabi, November 2011) [talk] [Canada]
120. Waterloo Chemical Physics Conference (Peter Limacher, November 2011) [poster] [Canada]
121. Department of Chemistry; Mount St. Vincent Univ. (Farnaz Heidarzadeh, Nov. 2011) [invited talk] [Canada]
122. University of Tokyo (Matthew Chan, Jan. 2012) [poster] [Japan]
123. Global Centers of Excellence Career Symposium (Matthew Chan, Jan. 2012) [invited talk] [Japan]

124. Current Research in Science and Technology (Farnaz Heidarzadeh, March 2012) [talk] [Canada]
125. Current Research in Science and Technology (Sandra Rabi, March 2012) [talk] [Canada]
126. Current Research in Science and Technology (Paul Johnson, March 2012) [talk] [Canada]
127. Challenges in Density Matrix and Density Functional Theory (Paul Johnson, April 2012) [poster][Belgium]
128. Challenges in Density Matrix and Density Functional Theory (Peter Limacher, April 2012) [poster][Belgium]
129. Division of Theoretical Chemistry, Vrije Universiteit Amsterdam (Paul Johnson, April 2012) [invited talk][Belgium]
130. Laboratoire de Chimie Theorique Appliquee, Facultes Universitaires Notre-Dame de la Paix, (Peter Limacher, April 2012) [invited talk][Belgium]
131. Inaugural Changsha Workshop on Theoretical and Computational Chemistry (James Anderson, June 2012) [invited talk][China]
132. 2nd Workshop on Sparse Grids and Applications (James Anderson, July 2012) [talk][Germany]
133. 25th Canadian Symposium on Theoretical and Computational Chemistry (Rogelio Cuevas, July 2012) [invited talk][Canada]
134. 25th Canadian Symposium on Theoretical and Computational Chemistry (James Anderson, July 2012) [invited talk][Canada]
135. 25th Canadian Symposium on Theoretical and Computational Chemistry (Paul Johnson, July 2012) [poster][Canada]
136. 25th Canadian Symposium on Theoretical and Computational Chemistry (Farnaz Heidarzadeh, July 2012) [poster][Canada]
137. 25th Canadian Symposium on Theoretical and Computational Chemistry (Peter Limacher, July 2012) [poster][Canada]
138. 25th Canadian Symposium on Theoretical and Computational Chemistry (Sandra Rabi, July 2012) [poster][Canada]
139. Sagamore XVII Workshop (James Anderson, July 2012) [poster][Japan]
140. Farnaz Heidar Zadeh, Swiss Chemical Society Meeting [poster][Switzerland] (Sept. 2012)
141. Farnaz Heidar Zadeh, Paul W. Ayers. CECAM Workshop on Machine Learning in Atomistic Simulations [poster][Switzerland]
142. Workshop on New Methods in Electronic Structure Theory (Farnaz Heidar Zadeh, October 2012) [invited talk][Belgium]
143. Waterloo Chemical Physics Conference (Farnaz Heidar Zadeh, November 2012) [poster] [Canada]
144. Waterloo Chemical Physics Conference (Santa Rabi, November 2012) [poster] [Canada]
145. Waterloo Chemical Physics Conference (Christopher Haddad, November 2012) [poster] [Canada]
146. Waterloo Chemical Physics Conference (Peter Limacher, November 2012) [talk] [Canada]
147. Waterloo Chemical Physics Conference (Paul Johnson, November 2012) [talk] [Canada]
148. Canadian Society for Chemistry Conference (Rogelio Cuevas, May 2013) [poster] [Canada]
149. Canadian Society for Chemistry Conference (Ahmed Mohammad, May 2013) [talk] [Canada]
150. Canadian Society for Chemistry Conference (James Anderson, May 2013) [talk] [Canada]
151. 7th Molecular Quantum Mechanics Meeting (Peter Limacher, June 2013) [talk] [Switzerland]
152. Applied Mathematics, Modelling, and Computational Science (AMMCS-2013) (Farnaz Heidar Zadeh, August 2013) [talk] [Canada]
153. Applied Mathematics, Modelling, and Computational Science (AMMCS-2013) (Cristina Gonzalez, August 2013) [talk] [Canada]
154. Applied Mathematics, Modelling, and Computational Science (AMMCS-2013) (Matt Chan, August 2013) [talk] [Canada]
155. Applied Mathematics, Modelling, and Computational Science (AMMCS-2013) (Pawel Tecmer, August 2013) [talk] [Canada]
156. Applied Mathematics, Modelling, and Computational Science (AMMCS-2013) (Farnaz Heidar Zadeh, August 2013) [talk] [Canada]
157. Applied Mathematics, Modelling, and Computational Science (AMMCS-2013) (Ahmed Mohammed, August 2013) [talk] [Canada]
158. Applied Mathematics, Modelling, and Computational Science (AMMCS-2013) (Peter Limacher, August 2013) [talk] [Canada]
159. Applied Mathematics, Modelling, and Computational Science (AMMCS-2013) (Kasia Boguslawski, August 2013)

[talk] [Canada]
160. Center for Molecular Modeling, Ghent University (Paul Johnson, September 2013) [invited talk] [Belgium]
161. DFT2013; 15th International Conference on the Theory and Applications of Density Functional Theory (Peter Limacher, August 2013) [talk] [England]
162. DFT2013; 15th International Conference on the Theory and Applications of Density Functional Theory (Taewon (David) Kim, August 2013) [poster] [England]
163. DFT2013; 15th International Conference on the Theory and Applications of Density Functional Theory (Matt Chan, August 2013) [poster] [England]
164. Ruhr-Universität, Bochum (Paul Johnson, October 2013) [invited talk] [Germany]
165. Advances in Quantum Chemical Topology (Farnaz Heidar Zadeh, October 2013) [invited talk] [Mexico]
166. Waterloo Chemical Physics Conference (Farnaz Heidar Zadeh, November 2013) [talk] [Canada]
167. Waterloo Chemical Physics Conference (Cristina Gonzalez, November 2013) [poster] [Canada]
168. Waterloo Chemical Physics Conference (Kasia Boguslawski, November 2013) [poster] [Canada]
169. Waterloo Chemical Physics Conference (Pawel Tecmer, November 2013) [poster] [Canada]
170. 8th international meeting on Mathematical Methods for Ab Initio Quantum Chemistry (Paul Johnson, November 2013) [poster][France]
171. 8th international meeting on Mathematical Methods for Ab Initio Quantum Chemistry (Kasia Boguslawski, November 2013) [poster][France]
172. 8th international meeting on Mathematical Methods for Ab Initio Quantum Chemistry (Pawel Tecmer, November 2013) [poster][France]
173. Symposium in Honor of Norman H. March (Paul Johnson, November 2013) [poster][Belgium]
174. Symposium in Honor of Norman H. March (Kasia Boguslawski, November 2013) [poster][Belgium]
175. Symposium in Honor of Norman H. March (Pawel Tecmer, November 2013) [poster][Belgium]
176. Canada Days Workshop (Paul Johnson, November 2013) [invited talk][Belgium]
177. Canada Days Workshop (Kasia Boguslawski, November 2013) [invited talk][Belgium]
178. Canada Days Workshop (Pawel Tecmer, November 2013) [invited talk][Belgium]
179. Meeting on Methods for Modeling Molecules and Materials (M4) (Paul Johnson, December 2013) [invited talk][Canada]
180. Meeting on Methods for Modeling Molecules and Materials (M4) (Kasia Boguslawski, December 2013) [invited talk][Canada]
181. Meeting on Methods for Modeling Molecules and Materials (M4) (Ahmed Mohammed, December 2013) [invited talk][Canada]
182. Meeting on Methods for Modeling Molecules and Materials (M4) (Pawel Tecmer, December 2013) [invited talk][Canada]
183. Meeting on Methods for Modeling Molecules and Materials (M4) (Cristina Gonzalez, December 2013) [poster][Canada]
184. Meeting on Methods for Modeling Molecules and Materials (M4) (Matt Chan, December 2013) [poster][Canada]
185. Current Research in Science and Technology (Cristina Gonzalez, March 2014) [talk] [Canada]
186. Deparment of Mathematics, University of Nice Sophia Antipolis (Paul Johnson, April 2014) [invited talk][France]
186. Low-Scaling and Unconventional Electronic Structure Theory Methods; Telluride Scientific Reseach Conference. (Paul Johnson, June 2014) [poster][U.S.A.]
187. Canadian Symposium on Theoretical and Computational Chemistry (Cristina Gonzalez, July 2014) [poster][Canada]
188. Canadian Symposium on Theoretical and Computational Chemistry (Taewon (David) Kim, July 2014) [poster][Canada]
189. Canadian Symposium on Theoretical and Computational Chemistry (Pawel Tecmer, July 2014) [poster][Canada]
190. Canadian Symposium on Theoretical and Computational Chemistry (Katharina Boguslawski, July 2014) [poster][Canada]
191. European Seminar on Computational Methods in Quantum Chemistry (Matt Chan, September 2014) [poster]

[Belgium]
192. New Approaches in Theoretical Chemistry (Matt Chan, October 2014) [invited talk] [Chile]
193. New Approaches in Theoretical Chemistry (Cristina Gonzalez, October 2014) [invited talk] [Chile]
194. New Approaches in Theoretical Chemistry (Farnaz Heidar Zadeh, October 2014) [invited talk] [Chile]
195. New Approaches in Theoretical Chemistry (Pawel Tecmer, October 2014) [invited talk] [Chile]
196. New Approaches in Theoretical Chemistry (Katharina Boguslawski, October 2014) [invited talk] [Chile]
197. World Association of Theoretically-Oriented Chemists (WATOC-2014) (Matt Chan, October 2014) [poster] [Chile]
198. World Association of Theoretically-Oriented Chemists (WATOC-2014) (Cristina Gonzalez, October 2014) [poster] [Chile]
199. World Association of Theoretically-Oriented Chemists (WATOC-2014) (Pawel Tecmer, October 2014) [poster] [Chile]
200. World Association of Theoretically-Oriented Chemists (WATOC-2014) (Katharina Boguslawski, October 2014) [poster] [Chile]
201. World Association of Theoretically-Oriented Chemists (WATOC-2014) (Farnaz Heidar Zadeh, October 2014) [poster] [Chile]
202. WATOC 2014 Satellite: Large Condensed and Biological Systems (Matt Chan, October 2014) [invited talk] [Chile]
203. WATOC 2014 Satellite: Large Condensed and Biological Systems (Cristina Gonzalez, October 2014) [invited talk] [Chile]
204. WATOC 2014 Satellite: Large Condensed and Biological Systems (Farnaz Heidar Zadeh, October 2014) [invited talk] [Chile]
205. WATOC 2014 Satellite: Large Condensed and Biological Systems (Pawel Tecmer, October 2014) [invited talk] [Chile]
206. Chemical Physics Theory Group Seminar; University of Toronto (Paul Johnson, October 2014) [invited talk] [Canada]
207. Department of Physics; Univ. of Chile (Farnaz Heidar-Zadeh, October 2014) [invited talk]
208. 8th Meeting on Photodynamics (Cristina Gonzalez, October 2014) [poster] [Mexico]
209. Waterloo Chemical Physics Conference (David Kim, November 2014) [poster] [Canada]
210. Waterloo Chemical Physics Conference (Sung Hong, November 2014) [poster] [Canada]
211. Waterloo Chemical Physics Conference (Corinne Duperrouzel, November 2014) [poster] [Canada]
212. Waterloo Chemical Physics Conference (Chunying Rong, November 2014) [poster] [Canada]
213. Waterloo Chemical Physics Conference (Yilin Zhang, November 2014) [poster] [Canada]
214. Waterloo Chemical Physics Conference (Kasia Boguslawski, November 2014) [poster] [Canada]
215. Waterloo Chemical Physics Conference (Pawel Tecmer, November 2014) [talk] [Canada]
216. Centro de Investigaciones Quimicas (CIQ), Universidad Autonoma del Estada de Morelos (UAEM) (Cristina Gonzalez, November 2014) [invited talk] [Mexico]
217. Dept. of Chemistry; Universidad Autonoma Metropolitana (UAM) (Cristina Gonzalez, December 2014) [invited talk] [Mexico]
218. Department of General Chemistry; Vrije Universiteit Brussel (Farnaz Heidar-Zadeh, January 2015) [invited talk] [Belgium]
219. Department of Chemistry, Syracuse University (Katharina Boguslawski, March 2015) [invited talk][U.S.A.]
220. Recent Advances in Electronic Structure Theory (Katharina Boguslawski, June 2015) [poster][China]
221. Recent Advances in Electronic Structure Theory (Pawel Tecmer, June 2015) [poster][China]
222. International Congress of Quantum Chemistry (Katharina Boguslawski, June 2015) [poster][China]
223. International Congress of Quantum Chemistry (Pawel Tecmer, June 2015) [poster][China]
224. International Congress of Quantum Chemistry (Ramon Miranda-Quintana, June 2015) [poster][China]
225. International Congress of Quantum Chemistry (Marco Franco-Perez June 2015) [poster][China]
226. International Congress of Quantum Chemistry (Chunying Rong, June 2015) [poster][China]
227. International Congress of Quantum Chemistry (Yilin Zhao, June 2015) [poster][China]
228. International Congress of Quantum Chemistry (Matthew Chan, June 2015) [poster][China]
229. International Congress of Quantum Chemistry (Farnaz Heidar-Zadeh, June 2015) [poster][China]

230. International Congress of Quantum Chemistry (Derrick Yang, June 2015) [poster][China]
231. International Congress of Quantum Chemistry (David Kim, June 2015) [poster][China]
232. Chemical Bonds at the 21st Century (Farnaz Heidar-Zadeh, June 2015) [poster][China]
233. Chemical Bonds at the 21st Century (David Kim, June 2015) [poster][China]
234. Novel computational methods for quantitative electronic structure calculations (Katharina Boguslawski, June 2015) [poster][Japan]
235. Novel computational methods for quantitative electronic structure calculations (Pawel Tecmer, June 2015) [poster][Japan]
236. Novel computational methods for quantitative electronic structure calculations (Marco Franco-Perez, June 2015) [poster][Japan]
237. Novel computational methods for quantitative electronic structure calculations (Matthew Chan, June 2015) [poster][Japan]
238. Congress of Theoretical Chemists of Latin Expression (QUITEL) (Cristina Gonzalez, July 2015) [poster][Italy]
239. 16th International Conference on Density Functional Theory and its Applications (Marco Franco, August 2015) [contributed talk][Hungary]
240. Laboratoire de Physique des Lasers, Atomes et Molécules, Lille (Sophie Kervazo,Oct. 2015) [invited talk][France]
241. Waterloo Chemical Physics Conference (David Kim, November 2015) [poster] [Canada]
242. Waterloo Chemical Physics Conference (Caitlin Lanssens, November 2015) [poster] [Canada]
243. Waterloo Chemical Physics Conference (Sophie Kervazo, November 2015) [poster] [Canada]
244. Waterloo Chemical Physics Conference (Derrick Yang, November 2015) [poster] [Canada]
245. Waterloo Chemical Physics Conference (Yilin Zhao, November 2015) [poster] [Canada]
246. Waterloo Chemical Physics Conference (Farnaz Heidar-Zadeh, November 2015) [poster] [Canada]
247. Waterloo Chemical Physics Conference (Michael Richer, November 2015) [poster] [Canada]
248. Waterloo Chemical Physics Conference (Kumru Dikmenli, November 2015) [poster] [Canada]
249. Waterloo Chemical Physics Conference (Anand Patel, November 2015) [poster] [Canada]
250. Waterloo Chemical Physics Conference (Cristina Gonzalez, November 2015) [poster] [Canada]
251. Waterloo Chemical Physics Conference (Matt Chan, November 2015) [poster] [Canada]
252. Pacifichem Conference (Pawel Tecmer, December 2015) [invited talk] [U.S.A.]
253. Pacifichem Conference (Kasia Boguslawski, December 2015) [invited talk] [U.S.A.]
254. Pacifichem Conference (Pawel Tecmer, December 2015) [contributed talk] [U.S.A.]
255. Virtual Winter School on Computational Chemistry (Ramon Miranda, Feb. 2016) [poster][online]
256. Virtual Winter School on Computational Chemistry (Ramon Miranda, Feb. 2016) [invited talk][online]
257. Chemistry Conference for Young Scientists (ChemCYS) (Farnaz Heidar-Zadeh, March 2016) [invited talk][Belgium]
258. Solvay Workshop on "Conceptual quantum chemistry: present aspects and challenges for the future" (Marco Franco, April 2016) [invited talk] [Belgium]
259. Solvay Workshop on "Conceptual quantum chemistry: present aspects and challenges for the future" (Cristina Gonzalez, April 2016) [poster] [Belgium]
260. Solvay Workshop on "Conceptual quantum chemistry: present aspects and challenges for the future" (Ramon Miranda, April 2016) [poster] [Belgium]
261. Solvay Workshop on "Conceptual quantum chemistry: present aspects and challenges for the future" (Farnaz Heidar-Zadeh, April 2016) [poster] [Belgium]
262. Western New York ACS Undergraduate Symposium (Anand Patel, Apr. 2016) [contributed talk][U.S.A]
263. CECAM Workshop on Exploring Chemical Space with Machine Learning and Quantum Mechanics (Farnaz Heidar-Zadeh, May 2016) [poster][Switzerland]
264. University at Buffalo Graduate Student Symposium (Anand Patel, May 2016) [contributed talk][U.S.A.]
265. University at Buffalo Graduate Student Symposium (Kumru Dikmenli, May 2016) [poster][U.S.A.]
266. International Symposium on Molecular Spectroscopy (Nike Dattani, June 2016) [contr. talk][U.S.A.]
267. International Symposium on Molecular Spectroscopy (Nike Dattani, June 2016) [contr. talk][U.S.A.]
268. International Symposium on Molecular Spectroscopy (Nike Dattani, June 2016) [contr. talk][U.S.A.]
269. International Symposium on Molecular Spectroscopy (Nike Dattani, June 2016) [contr. talk][U.S.A.]
270. Adiabatic Quantum Computing 2016 (Nike Dattani, June 2016) [contr. talk][U.S.A.]
271. International Workshop on Tensor Networks and Quantum Many-Body Problems (Yilin Zhao, July 2016) [poster][Japan]

272. International Symposium on Theoretical Chemical Physics (Sophie Kervazo, July 2016)[poster][U.S.A.]
273. Ghent Theoretical Chemistry Workshop (David Kim, October 2016) [invited talk][Belgium]
274. Ghent Theoretical Chemistry Workshop (Kumru Dikmenli, October 2016) [invited talk][Belgium]
275. Ghent Theoretical Chemistry Workshop (Michael Richer, October 2016) [invited talk][Belgium]
276. Ghent Theoretical Chemistry Workshop (Nike Dattani, October 2016) [invited talk][Belgium]
277. Ghent Theoretical Chemistry Workshop (Caitlin Lanssens, October 2016) [invited talk][Belgium]
278. Waterloo Symposium on Chemical Physics (Anand Patel, Nov. 2016) [poster][U.S.A.]
279. Waterloo Symposium on Chemical Physics (David Kim, Nov. 2016) [poster][U.S.A.]
280. Waterloo Symposium on Chemical Physics (Michael Richer, Nov. 2016) [poster][U.S.A.]
281. Waterloo Symposium on Chemical Physics (Stijn Fias, Nov. 2016) [poster][U.S.A.]
282. Waterloo Symposium on Chemical Physics (Derrick Yang, Nov. 2016) [poster][U.S.A.]
283. Waterloo Symposium on Chemical Physics (Cristina Gonzalez, Nov. 2016) [poster][U.S.A.]
284. Waterloo Symposium on Chemical Physics (Kumru Dikmenli, Nov. 2016) [poster][U.S.A.]
285. Excited State Simulations: Bridging Scales (Sophie Kervazo, Nov. 2016) [poster][France]
286. XV Reunión Mexicana de Fisicoquímica Teórica (Marco Franco, Nov. 2016) [poster][Mexico]
287. XV Reunión Mexicana de Fisicoquímica Teórica (Cristina Gonzalez, Nov. 2016) [contributed talk][Mexico]
288. XV Reunión Mexicana de Fisicoquímica Teórica (Matt Chan, Nov. 2016) [poster][Mexico]
289. XV Reunión Mexicana de Fisicoquímica Teórica (Marco Franco, Nov. 2016) [poster][Mexico]
290. Dept. of Chemistry, Universidad Autónoma del Estado de Morelos (Matt Chan, Nov. 2016) [invited talk][Mexico]
291. Dept. of Chemistry, Universidad Autónoma del Estado de Morelos (Cristina Gonzalez, Nov. 2016) [invited talk][Mexico]
292. Theoretical Chemistry Division, Cinvestav, Mexico City (Matt Chan, Nov. 2016) [invited talk][Mexico]
293. Theoretical Chemistry Division, Cinvestav, Mexico City (Cristina Gonzalez, Nov. 2016) [invited talk][Mexico]
294. Institute for Pure and Applied Mathematics, Univ. Calif. Los Angeles (Farnaz Heidar-Zadeh, Dec. 2016) [invited talk][U.S.A.]
295. GDR Colloquium, CNRS, Lille (Sophie Kervazo, Dec. 2016) [invited talk][France]
296. Virtual Winter School on Computational Chemistry (Ramon Miranda, Jan. 2017) [poster][online]
297. Quantum Information Processing (Nike Dattani, Jan. 2017) [poster][U.S.A.]

3. CITIZENSHIP

3.1 Member of the Editorial Board: ***THEOCHEM, Journal of Molecular Structure*****, 2009-2010**
Computational and Theoretical Chemistry **2011-**
The Scitech **(advisory board) 2012-**
Physical Chemistry Chemical Physics (advisory board) **2017-**

Editor of Special Issue of Computational and Theoretical Chemistry on "Density Matrices and Related Techniques" (in honor of A. John Coleman)

3.2 Member of the delegation from the Canadian Society for Chemistry to China, 2008

3.3 Member of National Science Foundation (U.S.) Study Session on Software Infrastructure for Scientific Innovation

3.4 Conference Organizer

231st National Meeting of the American Chemical Society "Frontier Applications and Developments of Density Functional Theory" (2006; Computational/Physical Divisions; co-organizer with W. Yang)
92nd Canadian Chemistry Conference and Exhibition, "Atoms in Molecules" (2009; co-organizer with Cherif Matta)
92nd Canadian Chemistry Conference and Exhibition, "Static Electron Correlation" (2009; co-organizer with Marcel Nooijen)
International Symposium on Molecular Dynamics and Reactivity (2010)
2nd International Symposium on Molecular Dynamics and Reactivity (2011)
3rd International Symposium on Molecular Dynamics and Reactivity (2011)
4th International Symposium on Molecular Dynamics and Reactivity (2011)

243rd National Meeting of the American Chemical Society "Theory and Applications of Density Functional Theory," (2012; Computational Division, co-organized with Weitao Yang)

65 Years in Quantum Chemistry; A Symposium in Honor of Prof. Robert G. Parr (2013; co-organized with Weitao Yang)

Applied Mathematics, Modelling, and Computational Science: "Density Functional Theory" (AMMCS-2013; Co-organized with Viktor Staroverov and Ian Hamilton)

M4 Meeting (Meeting on Methods for Modeling Molecules and Materials) (2013)

New Approaches in Theoretical Chemistry (DFT-Days) (Santiago, Chile) (2014) Co-organized with Carlos Cardenas.

Workshop on Quantum Marginals and Numerical Ranges (Guelph, Canada) (2015) (co-organized with David Kribs and Bei Zeng)

International Symposium on Theoretical Chemical Physics (Grand Forks, North Dakota) (2016) (co-organized with Pedro Salvador, Mark Hoffmann, and others)

Canadian Chemistry Conference and Exhibition (2017; co-organizer with Marcel Nooijen and Viktor Staroverov)

CECAM Meeting on Valence Bond Theory (2017; co-organizer with Benoit Braida, Wei Wu, and David Cooper)

Sagamore Meeting (2018, co-organizer with Cherif Matta)

International Conference on Density Functional Reactivity Theory (2018, co-organize with Shubin Liu)

4. TRAINING

High-School Co-op Students:

Sung-Min Lee (1/2007-8/2007)
Maria Tzoganakis (9/2015-1/2016)

Undergraduate Thesis Students:

Stuart Bothwell (10/2003-4/2004)
Sarah Rauscher (10/2003-4/2004)
Allison Chapman (10/2004-4/2005)
Sung Hong (9/2014-4/2015; Biology; McMaster University)
Karl Jobst (9/2005-4/2006) [co-supervised with Prof. Hans Terlouw]
Mathew Komorowski (9/2006-6/2007)
Michael Lacasse (9/2010-4/2011)
Sandra Rabi (9/2008-4/2009)
Nataly Rabi (9/2010-4/2011)
Ankit Rastogi (9/2010-4/2011)
Tyler Russell (9/2011-4/2012)
Abdul Shehata (9/2010-4/2011)
Ismat Sumar (9/2011-4/2012)
Christopher Haddad (8/2012-5/2013; Health Sciences, McMaster Univ.)
Santa Rabi (8/2012-5/2013; Health Sciences, McMaster University)
David Kim (8/2012-5/2013; Chemistry, McMaster Univ.)
Adam Mepham (8/2012-5/2013; Chemical Biology, McMaster University)
Phillip Daniel-Ivad (8/2013-5/2014; Chemical Biology; McMaster University)
Anand Patel (8/2015-5/2016; Chemical Biology; McMaster University)
Corinne Duperrouzel (8/2016-5/2017; Chemical Biology; McMaster University)

Undergraduate Students (Non-Thesis)

James S. M. Anderson (5/2003-8/2003; Chemistry, Queen's Univ.)
Marek Janicki (5/2003-8/2003; 5/2005-8/2005; Computer Science, Cornell Univ.)
Zobia Jawed (1/2003-10/2003; Health Sciences, McMaster Univ.)
Jordan Thomson (5/2004-8/2004; 5/2005-8/2005; Chemistry, McMaster Univ.)
Melissa Ng (6/2004-12/2004; Mathematics, McMaster Univ.)
Sarah Mansour (Rauscher) (5/2004-8/2004; Physics, McMaster Univ.)
Sandra Rabi (5/2006-8/2008; Chemistry, McMaster University)
Nataly Rabi (5/2008-8/2012; Chemistry, McMaster Univ.)
Marie Yan (5/2010-8/2010; Health Sciences; McMaster Univ.)
David Kim (5/2010-8/2010; Chemistry, McMaster Univ.)

Santa Rabi (5/2010-8/2012; Health Sciences, McMaster University)
Christopher Haddad (8/2011-8/2012; Health Sciences, McMaster Univ.)
Adam Mepham (1/2012-8/2012; Chemical Biology, McMaster University)
Sasha Mitchell (1/2012-5/2012; Life Sciences, McMaster University)
Bonnie Huang (1/2012-6/2012; Life Sciences, McMaster University)
Phillip Daniel-Ivad (5/2013-8/2013; Chemical Biology; McMaster University)
Luning Zhao (6/2013-9/2013; Chemical Engineering; Nanjing University)
Daniel Stuart (9/2014-12/2014; Chemistry Co-op; McMaster University)
Nicole Dumont (5/2014-8/2014, 5-2015-8/2015; 5/2016-7/2016; Physics; McMaster University)
Corinne Duperrouzel (5/2014-8/2014, 5-2015-8/2015; Chemistry; McMaster University)
Anand Patel (5/2014-8/2014, 5-2015-8/2015; Chemical Biology; McMaster University)
Jonathan La (5-2015-8/2015; Engineering Physics; McMaster University)
Tristan Goodwill (1/2016-5/2016; Integrated Science; McMaster Univ., co-supervised R. Dumont)
Michael Wang (1/2016-5/2016; Integrated Science; McMaster Univ., co-supervised R. Dumont)
Raisa Ahmed (3/2016-8/2016; MURSA)
Alireza Tehrani (5-2015-8/2015; 5/2016-present; Biochemistry & Mathematics; McMaster University)

Graduate Students:

James S. M. Anderson (2004-2010)
Debajit Chakraborty (2007-2011)
Matthew Chan (2011-present)
Rogelio Cuevas (2007-2012)
Kumru Dikmenli (2015-present)
Eleonora Echegaray (2008-present) [joint M.B.A./Ph.D.,with Alejandro Toro Labbe; PUC, Chile and EPFL Lausanne]
Cristina Gonzalez (2013-present)
Farnaz Heidazadeh (2010-present)
Richard Howell (2014, withdrawn)
Paul Johnson (2009-2014)
Sophie Kervazo (2015-present) [joint Ph.D. with Valerie Vallet at Univ. of Lille, France]
Taewon (David) Kim (5/2014-present)
Pavel Kulikov (2008; withdrawn)
Caitlin Lanssens (8/2015-5/2016) [joint M.Sc. with Patrick Bultinck at Ghent University]
Caitlin Lanssens (6/2016-present) [joint Ph.D. with Patrick Bultinck at Ghent University]
Yuli (Annie) Liu (2004-2011)
Fanwang Meng (2016-present)
Ramon Miranda Quintana (2013-2017) [with Prof. Luis Montero, Univ. of Havana]
Ahmed Mohammed (2009-2013, M.Sc.; 2013-present, Ph.D.)
Anand Patel (5/2016-present)
Sandra Rabi (2009-2014)
Michael Richer (2015-present)
Juan I. Rodriguez Hernandez (2003-2008)
Chunying Rong (2014-2016) [with Prof. Shubin Liu, Hunan Normal University]
Helen Van Aggelen (2007-2011) [with Patrick Bultinck and Dimitri Van Neck, Univ. of Ghent, Belgium]
Ivan Vinogradov (2005; withdrawn)
Xiaotian (Derrick) Yang (2014-present)
Yilin Zhang (2014-present)

Post-Doctoral Research Associates:

Katharina (Kasia) Boguslawski (7/2013-7/2015)
Steven Burger (9/2007 – 12/2011; co-supervised 1/2012-12/2012)
Carlos Cardenas (4/2008-4/2010)
Nike Dattani (6/2016-present)
Bijoy K. Dey (8/2003-3/2005;10/2005-2/2007)
Stijn Fias (11/2016-present)

Marco Franco Perez (11/2014-11/2016)
Alfredo Guevara (5/2009-6/2010)
Peter Limacher (1/2011-7/2014)
Lourdes Romero (5/2008 – 5/2009)
Utpal Sarkar (4/2006-6/2007)
Pawel Tecmer (7/2013-12/2015)
David Thompson (1/2004-4/2005)

5. OTHER CONTRIBUTIONS

5.1 Fellowships

Francis P. Venable Fellowship (1996-97,2000-01); *Charles N. Reilley Fellowship* (1996-97); *William Rand Kenan Jr. Fellowship* (1996-2001); *National Science Foundation Graduate Fellowship* (1996-2001); *National Institutes of Health Postdoctoral Research Fellowship* (2001-2002)

5.2 Awards & Other Recognition

Scholarship to the Kenneth Pitzer Symposium (2000)
Wiley International Journal of Quantum Chemistry Award (2002)
Research Innovation Award (Research Corp.) (2004)
Premier's Research Excellence Award (Ontario Government) (2004)
Alfred P. Sloan Fellowship (2008-2010)
Canadian Society for Chemistry "Best Student Chapter Award" (I was the advisor to the chapter) (2009)
Keith Laidler Award (Canadian Society for Chemistry; "for distinguished contribution to the field of physical chemistry while working in Canada. The award recognizes early achievement in the awardees independent research career.") (2011)
Acenet Lecture Series (2012)
Dirac Medal (World Association of Theoretically Oriented Chemists; "for the outstanding theoretical and computational chemist in the world under the age of 40") (2012)
Annual Medal of the International Academy of Quantum Molecular Science ("to a young member of the scientific community who has distinguished himself/herself by a pioneering and important contribution") (2012)
E. W. R. Steacie Memorial Fellowship ("to highly promising university faculty who are earning a strong international reputation for original research") (2013)
Steacie Prize for Natural Sciences ("for exceptional research contributions from a scientist or engineer aged 40 or younger") (2013)
Rutherford Memorial Medal from the Royal Society of Canada ("for outstanding research in physics and in chemistry") (2014)
Promising Scientist Award of the Centre de Mécanique Ondulatoire Appliquée (CMOA) (2014)
University Scholar (McMaster University) (2015-2019)
Elected to the College of Young Scholars of the Royal Society of Canada (2016)

5.3 Awards Won by Research Group Members

CONACYT Graduate Fellowship (Juan Rodriguez) (2003-2007)
1st year student research fellowship (Jordan Thomson) (2004)
Humboldt Fellowship (Bijoy K. Dey) (2005)
NSERC-Undergraduate Student Research Award (USRA) (Jordan Thomson) (2005)
NSERC-Undergraduate Student Research Award (USRA) (Marek Janicki) (2005)
Morrison Fellowship (James S. M. Anderson) (ca. $3,300) (2005-2006)
Mutual Group "Prestige" Fellowship (Yuli (Annie) Liu) (ca. $11,000 + teaching release) (2005-2006)
1st year student research fellowship (Sandra Rabi) (2006)
OGS-ST Fellowship (James S. M. Anderson) (2006-2007)
NSERC-Undergraduate Student Research Award (USRA) (Sandra Rabi) (2007)
CONACYT Graduate Fellowship (Rogelio Cuevas) (2007-2010)
NSERC-PGS graduate fellowship (James Anderson) (2007-2010)

Ontario Graduate Scholarship (OGS) (James Anderson) (2007; declined in lieu of NSERC-PGS)
E. B. Eastburn postdoctoral fellowship (Steven Burger) (2007-2009)
Chemical Computing Group Excellence Award (James Anderson) (2007)
Mutual Group "Prestige" Fellowship (Yuli (Annie) Liu) (ca. $11,000 + teaching release) (2007-2008)
Sharcnet Postdoctoral Fellowship (Carlo Cardenas) (2008-2010)
NSERC-Undergraduate Student Research Award (USRA) (Sandra Rabi) (2008)
CONACYT Postdoctoral Fellowship (Lourdes Romero) (2008-2009)
OGS-ST Fellowship (Annie Liu) (2008-2009)
Japan Society for Promotion of Science Study Abroad Grant (James Anderson) (2008)
Travel Fellowship for International Conference Odyssey (James Anderson) (2008)
Travel Fellowship for International Conference Odyssey (Rogelio Cuevas) (2008)
Graduate Studies Fellowship (for top first-year students in chemistry) (Rogelio Cuevas) (2008)
Japan Society for the Promotion of Science Postdoctoral Fellowship. (James Anderson) ('09-'10) [declined]
NSERC-Canada Graduate Scholarship (CGS-M) (Sandra Rabi) (2009-10)
Ontario Graduate Scholarship (OGS-M) (Sandra Rabi) (2009-10) [declined]
Ontario Graduate Scholarship (OGS-M) (Paul Johnson) (2009-10)
OGS-ST Fellowship (Annie Liu) (2008-2009)
NSERC-Undergraduate Student Research Award (USRA) (Paul Johnson) (2009)
Fields Institute Travel Award (James Anderson) (2009)
Fields Institute Travel Award (Rogelio Cuevas) (2009)
Fields Institute Travel Award (Pavel Kulikov) (2009)
Fields Institute Travel Award (Paul Johnson) (2009)
CONACYT Postdoctoral Fellowship (Alfredo Guevara) (2009-2010)
Sun Microsystems of Canada Scholarship in Computational Sciences and Engineering (Paul Johnson) (2009) [declined]
Outstanding Teaching Assistant Award (Ivan Vinogradov) (2009)
Outstanding Teaching Assistant Award (Rogelio Cuevas) (2009)
CONACYT Graduate Fellowship Extension (Rogelio Cuevas) (2009-2010)
NSERC Michael Smith Foreign Study Fellowship (Sandra Rabi) (2010)
NSERC PGS-D graduate fellowship (Sandra Rabi) (2010-2013)
OGS-D graduate fellowship (Sandra Rabi) (2010-2011) [declined]
NSERC CGS-M graduate fellowship (Paul Johnson) (2010-2011)
Ontario Graduate Scholarship (Paul Johnson) (2010-2011) [declined]
1st year student research fellowship (David Kim) (2010)
Health Sciences Undergraduate Research Award (Santa Rabi) (2010)
NSERC Michael Smith Foreign Study Fellowship (Paul Johnson) (2010)
James F. Harvey and Helen S. Harvey Travel Scholarship (James Anderson) (2010)
Japan Society for the Promotion of Science Postdoctoral Fellowship. (James Anderson) (2010-12)
Richard Fuller Science Fellowship (Rogelio Cuevas) (2010-11)
Swiss National Science Foundation Fellowship (Peter Limacher) (2010-2011)
Russell Bell Travel Award (Sandra Rabi) (2011)
McMaster Chemistry Graduate Colloquium award (Paul Johnson) (2010-11)
Russell Bell Travel Award (Paul Johnson) (2011, Greece)
OGS-M (Matthew Chan) (2011-2012)
OGS-M (Farnaz Heidarzadeh) (2011-2012)
Swiss National Science Foundation Fellowship (Peter Limacher) (2011-2012)
Outstanding Teaching Assistant Award (Farnaz Heidarzadeh) (Fall, 2011)
Vanier Canada Graduate Scholarship (Paul Johnson) (2011-2014)
NSERC Alexander Graham Bell Canada Graduate Scholarship (Paul Johnson) (2011-2014) [declined]
Global Centers of Excellence Travel Award (Matthew Chan) (2012; Japan)
Japan Society for the Promotion of Science Graduate Visit Fellowship. (Matt Chan) (2012)
Russell Bell Travel Award (Farnaz Heidarzadeh) (2012, Switzerland)
Russell Bell Travel Award (Sandra Rabi) (2012, U.S.A.)
Russell Bell Travel Award (Paul Johnson) (2012, Belgium)

NSERC-Undergraduate Student Research Award (USRA) (Adam Mepham) (2012)
NSERC postdoctoral fellowship (James Anderson) (2012-2014)
OGS-D (Farnaz Heidarzadeh) (2012-2013)
OGS-M (Matthew Chan) (2012-2013)
Best Poster Presentation Award, Swiss Chemical Society Meeting (Farnaz Heidar Zadeh) (2012)
1st prize, Departmental Colloquium Award (Farnaz Heidar Zadeh) (2012)
Cristina Gonzalez-Espinosa (CONACYT Ph.D. Fellowship) (2013-2016)
NSERC Alexander Graham Bell Canada Graduate Scholarship (Farnaz Heidar Zadeh) (2013-2016) [declined]
Vanier CGS Fellowship (Farnaz Heidar Zadeh) (2013; ranked #2 in Canada)
NSERC Michael Smith Foreign Study Fellowship (Farnaz Heidar Zadeh) (2013)
NSERC-Undergraduate Student Research Award (USRA) (Philip Daniel-Ivad) (2013)
School of Graduate Studies Grant in Aid of Travel Research & Field Study Fund (Paul Johnson) (2013)
Swiss National Science Foundation Postdoctoral Fellowship (Katharina Boguslawski) (2013)
Swiss National Science Foundation Postdoctoral Fellowship (Peter Limacher) (2014)
NSERC CGS-D graduate fellowship (Matthew Chan) (2014-2017)
1st year student research fellowship (Corinne Duperrouzel) (2014)
MITACS-France Globalink Research Award (Cristina Gonzalez) (2014)
MITACS Graduate Student Fellowship (Yilin Zhang) (2014-15)
National Science Foundation of China Foreign Fellowship (Chunying Rong) (2014-2015)
Emerging Leaders of the Americas Program (Ramon Miranda Quintana) (2015)
CONACYT Postdoctoral Fellowship (Mexico) (Marco Franco Perez) (2014-2015)
Banting Postdoctoral Fellowship (Canada) (Katharina Boguslawski) (2015)
NSERC Undergraduate Student Research Award (Corinne Duperrouzel) (2015)
Best Poster Prize; International Congress of Quantum Chemisry (Farnaz Heidar Zadeh) (2015)
Visiting Scholar Fund, Ghent University (2015)
CONACYT Postdoctoral Fellowship (Mexico) (Marco Franco Perez) (2015-2016)
MITACS Globalink Graduate Fellowship (Yilin Zhao) (2015-2016)
International Excellence Award, McMaster University (Kumru Dikmenli) (2015)
Most Outstanding Young Researcher (Univ. of Havana) (Ramon Miranda) (2015)
Marie Curie Postdoctoral Fellowship (Stijn Fias) (2016-2019)
Banting Postdoctoral Fellowship (Nike Dattani) (2016-2018)
Ontario Graduate Scholarship (Anand Patel) (2016)
Michael Smith Foreign Study Supplement (Matt Chan) (2016)
International Excellence Award, McMaster University (Ahmed Mohammed) (2016)
International Excellence Award, McMaster University (Kumru Dikmenli) (2016)
International Excellence Award, McMaster University (Cristina Gonzalez) (2016)
International Excellence Award, McMaster University (Derrick Yang) (2016)
MITACS Globalink Graduate Fellowship (Yilin Zhao) (2016-2017)
International Excellence Award, McMaster University (Yilin Zhao) (2016)
CONACyT Graduate Fellowship (Extension) (Cristina Gonzalez) (2016-2017)
China Council Graduate Scholarship (Fanwang Meng) (2016-2019)
Ontario Graduate Scholarship (Fanwang Meng) (2016-2017)
Best Poster Prize at the Winter School on Computational Chemistry (Farnaz Heidar-Zadeh) (2016)
Best Paper in the Natural and Exact Sciences (Univ. of Havana) (Ramon-Miranda) (2016)
Outstanding Research Activities (Univ. of Havana, a competition including all *faculty*) (Ramon Miranda) (2016)
Most Outstanding Young Researcher (Univ. of Havana) (Ramon Miranda) (2016)
Emerging Leaders of the Americas Program (Gabriela Garcia Munoz) (2017)

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