

Curriculum Vitae

Paul W. Ayers

June 4, 2010

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

Fellowships:

First Year Fellowships: Francis P. Venable Fellowship

Charles N. Reilley Fellowship

Three Year Fellowships: National Science Foundation Graduate Fellowship

William Rand Kenan Jr. Fellowship

Postdoctoral Associate (2001-2002): Department of Chemistry; Duke University (U.S.A.)

Supervisor: Weitao Yang

Fellowships: National Institutes of Health Postdoctoral Research Fellowship

Assistant Prof. (2002-); Associate Prof. (July 1, 2007-present): Dept. of Chemistry; McMaster Univ.
Canada Research Chair in Theoretical Chemistry and Chemical Biology (Tier 2) (2002-present)

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 analysis⁸ 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 algorithmic¹⁵ 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} Now, together with my collaborators, I am studying 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 fixed¹⁹ by enforcing stronger N -representability conditions (like the “sharp P ” and “sharp Q ” conditions I had previously derived¹⁴) or by using “wavefunction information” to induce a derivative discontinuity (as in Kohn-Sham DFT). I am supervising graduate students working on both approaches. Arguably the biggest problem, however, is the computational inefficiency of these methods; this is my individual focus.

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.

2. Research Contributions

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: (citations from ISI journals only, from *Web of Science*, corrected for typographical miscitations)

	< 2005	2005	2006	2007	2008	2009	2010	Accepted	Submitted
book chapters	1	0	0	1	0	3	1	0	1
journal articles	27	14	15	25	11	26	7	4	6
conference proceedings	0	0	0	4	0	0	0	0	0
single-author pubs.	4	4	5	3	2	1	0	0	1
first-author pubs.	12	5	4	8	2	5	0	0	2
collaborative pubs.	12	9	7	19	8	20	5	1	3
invited contributions	5	1	0	2	0	4	2	2	0
total publications (in each year)	28	14	15	30	11	29	8	4	7
citations (from papers published in this year)	286	137	183	452	437	594	29 (to 1/22)	h-index: 26	

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 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.
3. 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]
4. 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.
5. 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.
6. 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.
7. 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.
8. 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).
9. 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).
10. Agnes Nagy, Mel Levy, and Paul W. Ayers "Time-Independent Theories for a Single Excited State," in Theory of Chemical Reactivity; in Chemical Reactivity Theory: A Density Functional View; P. Chattaraj, Editor (Taylor and Francis, Boca Raton, 2009).

11. 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).

Book Reviews:

1. Paul W. Ayers, Advances in Quantum Chemistry, Volume 48. *J. Am. Chem. Soc.* **128**, 3468-3469 (2006).

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 H₂”; *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).
27. Paul W. Ayers, James S. M. Anderson, and Libero J. Bartolotti, "Perturbative Perspectives on the Chemical Reaction Prediction Problem"; *Int. J. Quantum Chem.* **101**, 520-534 (2005).
28. Libero J. Bartolotti and Paul W. Ayers, "An example where orbital relaxation is an important contribution to the Fukui function"; *J. Phys. Chem. A* **109**, 1146-1151 (2005).
29. Paul W. Ayers, James S. M. Anderson, Juan I. Rodriguez Hernandez, and Zobia Jawed, "Indices for Predicting the Quality of Leaving Groups"; *Phys. Chem. Chem. Phys.* **7**, 1918-1925 (2005).
30. Paul W. Ayers, "Generalized Density Functional Theories Using the k -electron Densities: Development of Kinetic-Energy Functionals"; *J. Math. Phys.* **46**, 062107 (pp. 1-22) (2005).
31. Robert G. Parr, Paul W. Ayers, and Roman F. Nalewajski "What Is An Atom in A Molecule"; *J. Phys. Chem. A* **109**, 3957-3959 (2005).
32. *Dina Tleugabulova*, *Jie Sui*, Paul W. Ayers and John D. Brennan, "Evidence for Rigid Binding of Rhodamine 6G to Silica Surfaces in Aqueous Solution based on Fluorescence Anisotropy Decay Analysis"; *J. Phys. Chem. B* **109**, 7850-7858 (2005).
33. Paul W. Ayers "An elementary derivation of the hard/soft acid/base principle"; *J. Chem. Phys., Communication* **122**, 141102 (pp. 1-3) (2005).
34. Paul W. Ayers, Robert C. Morrison, and Robert G. Parr, "Fermi-Amaldi Model for Exchange-Correlation: Atomic Excitation Energies from Orbital Energy Differences"; *Mol. Phys.* **103**, 2061-2072 (2005).
35. Paul W. Ayers, "Proof-of-Principle Functionals for the Shape Function"; *Phys. Rev. A* **71**, 062506 (pp. 1-8) (2005).
36. Pratim K. Chattaraj and Paul W. Ayers, "The Maximum Hardness Principle Implies the Hard/Soft Acid/Base Rule"; *J. Chem. Phys.* **123**, 086101 (pp. 1-2) (2005).
37. *Junia Melin*, Paul W. Ayers, and J. V. Ortiz, "The Electron-Propagator Approach to Conceptual Density-Functional Theory"; *J. Chem. Sci.* **117**, 387-400 (2005).
38. Paul W. Ayers, "Electron Localization Functions and Local Measures of the Covariance"; *J. Chem. Sci.* **117**, 441-454 (2005).
39. Paul W. Ayers and Mel Levy, "Generalized Density-Functional Theory: Conquering the N -representability Problem with Exact Functionals for the Electron Pair Density and the Second-Order Reduced Density Matrix"; *J. Chem. Sci.* **117**, 507-514 (2005).

40. Paul W. Ayers and Mel Levy, "Using the Kohn-Sham Formalism in Pair Density-Functional Theories"; *Chem. Phys. Lett.* **415**, 211-216 (2005).
41. David C. Thompson and Paul W. Ayers, "Thinking inside the box: A novel linear-scaling algorithm for Coulomb potential evaluation"; *Int. J. Quantum Chem.* **106**, 787-794 (2006).
42. Paul W. Ayers, "Axiomatic Formulations of the Hohenberg-Kohn Functional"; *Phys. Rev. A* **73**, 012513 (pp. 1-12) (2006).
43. Bijoy K. Dey and Paul W. Ayers, "A Hamilton-Jacobi Type Equation for Computing Minimum Potential Energy Paths"; *Mol. Phys.* **104**, 541-558 (2006).
44. Paul W. Ayers, Sidney Golden, and Mel Levy, "Generalizations of the Hohenberg-Kohn theorem"; *J. Chem. Phys.* **124**, 054101 (pp. 1-7) (2006).
45. David C. Thompson, Yuli Liu, and Paul W. Ayers "A Confined Noninteracting Many-Electron System: Accurate Corrections to a Statistical Model"; *Physics Letters A* **351**, 439-445 (2006).
46. Paul W. Ayers and Ernest R. Davidson, "Necessary Conditions for the N -representability of Pair Distribution Functions"; *Int. J. Quantum Chem.* **106**, 1487-1498 (2006).
47. Paul W. Ayers, "Density Bifunctional Theory Using the Mass Density and the Charge Density"; *Theor. Chem. Acc.* **115**, 253-256 (2006).
48. Paul W. Ayers, Robert G. Parr, and Ralph G. Pearson, "Describing Hard/Soft Acid/Base Exchange Using Half-Reactions" *J. Chem. Phys.* **124**, 194107 (pp. 1-8) (2006).
49. Paul W. Ayers, "Information Theory, the Shape Function, and the Hirshfeld Atom"; *Theor. Chem. Acc.* **115**, 370-378 (2006).
50. Paul W. Ayers and Weitao Yang "Legendre Transform Functionals for Spin Density Functional Theory"; *J. Chem. Phys.* **124**, 224108 (pp. 1-15) (2006).
51. Paul W. Ayers, "Can One Oxidize an Atom by Reducing the Molecule that Contains It?"; *Phys. Chem. Chem. Phys.* **8**, 3387-3390 (2006).
52. D. Van Neck, *S. Verdonck*, *G. Bonny*, P. W. Ayers, and M. Waroquier, "Quasiparticle Properties in a Density Functional Framework", *Phys. Rev. A* **74**, 042501 (pp. 1-9) (2006).
53. Paul W. Ayers "Using the Classical Many-Body Structure to Determine Electronic Structure: An Approach Using k -electron Distribution Functions", *Phys. Rev. A* **74**, 042502 (pp. 1-12) (2006).
54. Frank De Proft, Paul W. Ayers, *Stijn Fias*, and Paul Geerlings, "Woodward-Hoffmann rules in Conceptual Density Functional Theory : Initial Hardness Response and Transition State Hardness"; *J. Chem. Phys.* **125**, 214101 (pp. 1-9) (2006).
55. *S. Verdonck*, D. Van Neck, P. W. Ayers, and M. Waroquier, "Characterization of the Electron Propagator with a GW -like Selfenergy in Closed-Shell Atoms" *Phys. Rev. A* **74**, 062503 (pp. 1-14) (2006).
56. Paul W. Ayers "The Physical Basis of the Global and Local Hard/Soft Acid/Base Principles", *Faraday Discussions* **135**, 161-190 (2007).
57. Paul W. Ayers, Frank De Proft, and Paul Geerlings, "A Comparison of the Utility of the Shape Function and Electron Density for Predicting Periodic Properties: Atomic Ionization Potentials"; *Phys. Rev. A* **75**, 012508 (pp. 1-8) (2007).
58. *Tim Heaton-Burgess*, Paul W. Ayers, and Weitao Yang, "Spin-Potential Functional Formalism for Current Carrying Noncollinear Magnetic Systems", *Phys. Rev. Lett.* **98**, 036403 (pp. 1-4) (2007).
59. Bijoy K. Dey, Stuart Bothwell, and Paul W. Ayers, "Fast-Marching Method for Computing Reactive Trajectories for Chemical Reactions"; *J. Math. Chem.* **41**, 1-25 (2007).
60. Paul W. Ayers and Shubin Liu, "Necessary and Sufficient Conditions for the N -representability of Density Functionals", *Phys. Rev. A* **75**, 022504 (pp. 1-12) (2007).
61. Dimitri Van Neck and Paul W. 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 (pp. 1-6) (2007).

62. Paul W. Ayers and *Junia Melin*, "Computing the Fukui Function from *Ab Initio* Quantum Chemistry: Approaches Based on the Extended Koopmans' Theorem", *Theor. Chem. Acc.* **117**, 371-381 (2007).
63. James S. M. Anderson, *Junia Melin*, and Paul W. Ayers, "Conceptual Density-Functional Theory for General Chemical Reactions, Including Those That Are Neither Charge Nor Frontier-Orbital Controlled. I. Theory and Derivation of a General-Purpose Reactivity Indicator", *J. Chem. Th. Comp.* **3**, 358-374 (2007).
64. James S. M. Anderson, *Junia Melin*, and Paul W. Ayers, "Conceptual Density-Functional Theory for General Chemical Reactions, Including Those That Are Neither Charge Nor Frontier-Orbital Controlled. II. Application to Molecules Where Frontier Molecular Orbital Theory Fails"; *J. Chem. Th. Comp.* **3**, 375- 389(2007).
65. Paul W. Ayers "Using Reactivity Indices Instead of the Electron Density to Describe Coulomb Systems", *Chem. Phys. Lett.* **438**, 148-152 (2007).
66. Robert C. Morrison, Paul W. Ayers, and Agnes Nagy, "Density Scaling and Relaxation of the Pauli Principle"; *J. Chem. Phys.* **126**, 124111 (pp. 1-7) (2007).
67. Paul W. Ayers and Agnes Nagy, "Alternatives to the Electron Density for Describing Coulomb Systems", *J. Chem. Phys.* **126**, 144108 (pp. 1-6) (2007).
68. Patrick Bultinck, Christian Van Alsenoy, Paul W. Ayers, and Ramon Carbó-Dorca, "A Critical Analysis of the Hirshfeld Atom in a Molecule"; *J. Chem. Phys.* **126**, 144111 (pp. 1-9) (2007).
69. Bijoy K. Dey and Paul W. Ayers "Computing Tunneling Paths with the Hamilton-Jacobi Equation and the Fast-Marching Method"; *Mol. Phys.* **105**, 71-83 (2007).
70. James S. M. Anderson and Paul W. Ayers, "Predicting the Chemical Reactivity of Ambidentate Electrophiles and Nucleophiles Using a Single General-Purpose Reactivity Indicator", *Phys. Chem. Chem. Phys.* **9**, 2371-2378 (2007).
71. Paul W. Ayers and Ernest R. Davidson, "Linear Inequalities for Diagonal Elements of Density Matrices" *Advances in Chemical Physics* **134**, 443-483 (2007).
72. Paul W. Ayers, Frank De Proft, *Alex Borgoo*, and Paul Geerlings, "Computing the Fukui Function Without Differentiation with Respect to Particle Number. I. Basic Theory" *J. Chem. Phys.* **126**, 224107 (pp. 1-13) (2007).
73. *Nick Y. J. Sablon*, Frank De Proft, Paul W. Ayers, and Paul Geerlings, "Computing the Fukui Function Without Differentiation with Respect to Particle Number. II. Application: Calculation of condensed Fukui functions without finite difference approach" *J. Chem. Phys.* **126**, 224108 (pp. 1-6) (2007).
74. *T. Verstaelen*, 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"; *J. Chem. Th. Comp.* **3**, 1420-1434 (2007).
75. Pratim K. Chattaraj, Paul W. Ayers, and *Junia Melin*, "Further Links Between the Maximum Hardness Principle and the Hard/Soft Acid/Base Principle: Insights from Hard/Soft Exchange Reactions", *Phys. Chem. Chem. Phys.* **9**, 3853-3856 (2007).
76. Patrick Bultinck, *Stijn Fias*, Christian Van Alsenoy, Paul W. Ayers, and Ramon Carbó-Dorca, "Critical Thoughts on Computing Atom Condensed Fukui Functions", *J. Chem. Phys.* **127**, 034102 (pp. 1-11) (2007).
77. Paul W. Ayers, "On the Electronegativity Nonlocality Paradox"; *Theor. Chem. Acc.* **118**, 371-381 (2007).
78. Patrick Bultinck, Paul W. Ayers, *Stijn Fias*, *Koen Tiels*, and Christian Van Alsenoy, "Uniqueness and Basis set Dependence of Iterative Hirshfeld Charges" *Chem. Phys. Lett.* **444**, 205-208 (2007).
79. Paul W. Ayers, *Christophe Morell*, Frank De Proft, and Paul Geerlings "Understanding the Woodward-Hoffmann Rules Using Changes in the Electron Density. (No Orbitals Necessary.)" *Chemistry, A European Journal* **13**, 8240-8247 (2007).

80. *Junia Melin*, Paul W. Ayers, and Joseph Vincent Ortiz “Removing Electrons Can Increase the Electron Density in a Chemical Bond: A Computational Study of Negative Fukui Functions”, *J. Phys. Chem. (Letter)* **111**, 1017-1019 (2007).
81. Paul W. Ayers, “The Continuity of the Energy and Other Molecular Properties with Respect to the Number of Electrons”, *J. Math. Chem.* **43**, 285-303 (2008).
82. F. De Proft, P. K. Chattaraj, P. W. Ayers, M. Torrent-Sucarat, M. Elango, V. Subramanian, S. Giri, and P. Geerlings, “Initial Hardness Response and Hardness Profiles in the Study of Woodward-Hoffmann Rules for Electrocyclizations” *J. Chem. Theor. Comp.* **4**, 595-602 (2008).
83. Paul W. Ayers and Robert G. Parr, “Local Hardness Equalization: Exploiting the Ambiguity” *J. Chem. Phys.* **128**, 184108 (pp. 1-8) (2008).
84. Patricia Perez, Eduardo Chamorro, and Paul W. Ayers “Some Relationships Within the $[N_{\alpha}, N_{\beta}, \nu(\mathbf{r})]$ Representation of Spin Polarized Density Functional Theory” *J. Chem. Phys.* **128**, 204108 (pp. 1-22) (2008).
85. Juan I. Rodriguez, David C. Thompson, Paul W. Ayers, and Andreas Köster “Numerical Integration of Exchange-Correlation Energies and Potentials Using Transformed Sparse Grids”, *J. Chem. Phys.* **128**, 224103 (pp. 1-10) (2008).
86. Paul W. Ayers, “Constraints for Hierarchies of Many-Electron Distribution Functions;” *J. Math. Chem.* **44**, 311-323 (2008).
87. *T. Fievez*, *N. Sablon*, F. De Proft, P. W. Ayers, and P. Geerlings, “Calculation of Fukui Function without Differentiating with Respect to the Number of Electrons. Part III. Local Fukui Function and Dual Descriptor”, *J. Chem. Th. Comp.* **4**, 1065-1072 (2008).
88. Juan I. Rodriguez, David C. Thompson, James Anderson, Jordan Thomson, and Paul W. Ayers, “A Physically Motivated Pseudo-Gaussian Quadrature Scheme with Applications for Molecular Density Functional Theory” *J. Phys. A* **41**, 365202 (pp. 1-18) (2008).
89. Paul W. Ayers and Robert G. Parr, “Beyond the Electronegativity and the Local Hardness: Higher-Order Equalization Criteria for the Determination of the Ground-State Electron Density”, *J. Chem. Phys.* **129**, 054111 (pp. 1-7) (2008).
90. *M. Torrent-Sucarrat*, F. De Proft, P. Geerlings, and P. W. Ayers, “Do the Local Softness and Hardness Indicate the Softest and Hardest Regions of a Molecule?” *Chem. Eur. J.* **14**, 8652-8660 (2008).
91. *Christophe Morell*, André Grand, Alejandro Toro-Labbé, and Paul W. Ayers “Rationalization of Diels-Alder Reactions Through the Use of the $\Delta f(r)$ Descriptor”, *Phys. Chem. Chem. Phys.* **10**, 7239-7246 (2008).
92. Steven K. Burger, Yuli Liu, Utpal Sarkar, and Paul W. Ayers, “Moving Least-Squares Interpolation for the Fast-Marching and String Methods,” *J. Chem. Phys.* **130**, 024103 (pp. 1-8) (2009). [Selected for and published in the *Virtual Journal of Biological Physics Research*.]
93. *Matthew J. Swadley*, Paul W. Ayers, Shubin Liu, *Clare Aubrey-Medendorp*, and Tonglei Li “Molecular Packing and Polymorphism of 5-Methyl-2-[(2-nitrophenyl)amino]-3-thiophenecarbonitrile: Insights from Conceptual Density Functional Theory”, *Chem. Eur. J* **15**, 361-371 (2009).
94. S. Jenkins, P.W. Ayers, S.R. Kirk, *P. Mori-Sánchez* and A. Martín. Pendás, “Bond metallicity of materials from real space charge density distributions” *Chem. Phys. Lett.* **471**, 174-177 (2009).
95. Juan I. Rodríguez, Richard F. W. Bader, Paul W. Ayers, *Carine Michel*, Andreas W. Götz, and Carles Bo, “A High Performance Grid-Based Algorithm for Computing QTAIM Properties,” *Chem. Phys. Lett.* **472**, 149-152 (2009).
96. Paul W. Ayers, “A Perspective on the Link Between the Exchange(-Correlation) Hole and Dispersion Forces”, *J. Math. Chem.* **46**, 86-96 (2009).
97. Paul W. Ayers and Samantha Jenkins, “An Electron-Preceding Perspective on the Deformation of Materials”, *J. Chem. Phys.* **130**, 154104 (2009).

98. *Diederik Vanfleteren*, Dimitri Van Neck, Paul W. Ayers, Robert C. Morrison, and Patrick Bultinck, "Exact Ionization Potentials from Wavefunction Asymptotics: The Extended Koopmans' Theorem, Revisited", *J. Chem. Phys.* **130**, 194104 (pp. 1-10) (2009).
99. *Rogelio Cuevas-Saavedra* and Paul W. Ayers, "Coordinate scaling of the kinetic energy in pair density functional theory: A Legendre transform approach," *Int. J. Quantum Chem.* **109**, 1699-1705 (2009).
100. *Juan I. Rodriguez*, Andreas M. Koster, Paul W. Ayers, *Ana Santos-Valle*, *Gabriela Vera*, Gabriel Merino, and Alberto Vela, "An Efficient Grid-Based Scheme to Compute QT-AIM Properties Without Explicit Calculation of Zero-Flux Surfaces", *J. Comp. Chem.* **30**, 1082-1092 (2009).
101. *Soumen Saha*, Ram K. Roy, Kimihiko Hirao, and Paul W. Ayers, "Are the Hirshfeld and Mulliken Population Analysis Schemes Consistent with Chemical Intuition"; *Int. J. Quantum Chem.* **109**, 1780-1806 (2009).
102. Mel Levy and Paul W. Ayers, "Kinetic energy from a single Kohn-Sham orbital," *Phys. Rev. A* **79**, 064504 (pp. 1-2) (2009).
103. *Carlos Cárdenas*, *Eleonora Echegaray*, *Debajit Chakraborty*, *James S. M. Anderson*, and *Paul W. Ayers*, "Relationships Between the Third-Order Reactivity Indicators in Chemical Density-Functional Theory" *J. Chem. Phys.* **130**, 244105 (pp. 1-9) (2009).
104. Paul W. Ayers and Mel Levy "Time-Independent Density-Functional Theories for Pure Excited States: Extension and Unification" *Phys. Rev. A* **80**, 012508 (pp. 1-16) (2009).
105. *İlke Uğur*, *Freija De Vleeschouwer*, *Nurcan Tüzün*, *Viktorya Aviyente*, Paul Geerlings, Shubin Liu, Paul W. Ayers, and Frank De Proft, "Cyclopolymerization Reactions of Diallyl Monomers: Exploring Electronic and Steric Effects using DFT Reactivity Indices," *J. Phys. Chem. A* (accepted).
106. *Juan I. Rodríguez*, Paul W. Ayers, Andreas W. Götz, and F. L. Castillo-Alvarado, "Virial Theorem in the Kohn-Sham DFT Formalism: Accurate Calculation of the Atomic QTAIM Energies," *J. Chem. Phys.* **131**, 021101 (pp. 1-4) (2009).
107. *Carlos Cardenas*, *Nataly Rabi*, Paul W. Ayers, Christophe Morrel, *Paula Jaramillo*, and Patricio Fuentealba "Chemical Reactivity Descriptors for Ambiphilic Reagents: Dual Descriptor, Local Hypersoftness, and Electrostatic Potential", *J. Phys. Chem. A* **113**, 8660-8667 (2009).
108. *B. Verstichel*, *Helen Van Aggelen*, Dimitri Van Neck, Paul W. Ayers, and Patrick Bultinck "Variational determination of the second-order density matrix for the isoelectronic series of beryllium, neon, and silicon," *Phys. Rev. A* **80**, 032508, (pp. 1-14) (2009).
109. *Helen Van Aggelen*, Patrick Bultinck, *Brecht Verstichel*, Dimitri Van Neck and Paul W. Ayers, "Incorrect Diatomic Dissociation in Variational Reduced Density Matrix Theory Arises from the Flawed Description of Fractionally Charged Atoms", *Phys. Chem. Chem. Phys. (Communication)* **11**, 5558-5560 (2009).
110. Christophe Morell, *Vanessa Labet*, André Grand, Paul W. Ayers, Frank De Proft, Paul Geerlings, and Henry Chermette, "Characterization of the Chemical Behaviour of the Low Excited States through a Local Chemical Potential", *J. Chem. Th. Comp.* **5**, 2274-2283 (2009).
111. Paul W. Ayers and Patricio Fuentealba, "Density-Functional Theory with Additional Basic Variables: The Extended Legendre Transform", *Phys. Rev. A* **80**, 032510 (2009).
112. Shubin Liu, Tonglei Li, and Paul W. Ayers, "Potentialphilicity and Potentialphobicity: Reactivity Indicators for External Potential Changes from Density Functional Reactivity Theory", *J. Chem. Phys.* **131**, 114106 (pp. 1-7) (2009).
113. Paul W Ayers, Shubin Liu, and Tonglei Li, "Chargephilicity and Chargephobicity: Two New Reactivity Indicators for External Potential Changes from Density Functional Reactivity Theory", *Chem. Phys. Lett.* **480**, 318-321 (2009).
114. *T. Gal*, P. W. Ayers, F. De Proft, and P. Geerlings, "Nonuniqueness of Magnetic Fields and Energy Derivatives in Spin-Polarized Density Functional Theory," *J. Chem. Phys.* **113**, 154114 (2009).

115. Qin Wu, Paul W. Ayers, and Yingkai Zhang, "Density-based energy decomposition analysis for intermolecular interactions with variationally optimized intermediate state energies", *J. Chem. Phys.* **131**, 164112 (2009).
116. Bijoy K. Dey and Paul W. Ayers, "Computing the Chemical Reaction Path with a Ray-Based Fast Marching Technique for Solving the Hamilton-Jacobi equation in a General Coordinate System"; *J. Math. Chem.* **45**, 981-1003 (2009).
117. Paul W. Ayers and Juan I. Rodriguez, "Out of One, Many: Using Moment Expansions of the Virial Relation to Deduce Universal Density Functionals from a Single System," *Can. J. Chem.* (Ziegler Issue) **87**, 1540-1545 (2009). [invited article]
118. *M. Torrent-Sucarrat*, F. De Proft, Paul W. Ayers, and P. Geerlings, "On the Applicability of the Local Hardness and Softness", *Phys. Chem. Chem. Phys.* **12**, 1072-1080 (2010).
119. James S. M. Anderson, Yuli Liu, Jordan W. Thomson, and Paul W. Ayers "Predicting the Quality of Leaving Groups in Organic Chemistry: Tests Against Experimental Data", *THEOCHEM* **943**, 168-177 (2010). [invited article].
120. *B. Verstichel*, *Helen Van Aggelen*, Dimitri Van Neck, Paul W. Ayers, and Patrick Bultinck, "Subsystem Constraints in Variational Second Order Reduced Density Matrix Optimization: Curing Size Inconsistency", *J. Chem. Phys.* **132**, 114113 (2010).
121. *Helen Van Aggelen*, *Brecht Verstichel*, Patrick Bultinck, Dimitri Van Neck, Paul W. Ayers, and David L. Cooper, "Chemical Verification of Variational Second-Order Density Matrix Based Potential Energy Surfaces for the N₂ Isoelectronic Series." *J. Chem. Phys.* **132**, 114112 (2010).
122. C. Morell, *V. Labet*, P. W. Ayers, *N. L. Jorge*, and A. Grand, "Extending the 'Grochala-Albrecht-Hoffmann Approximation' to the Determination of the First Excited State Potential Energy Profile of a Reaction Step," *Chem. Phys. Lett.* **485**, 371-375 (2010).
123. Steven Burger and Paul W. Ayers, "Dual Grid Methods for Finding the Reaction Path on Reduced Potential Energy Surfaces", *Journal of Chemical Theory and Computation* **6**, 1490-1497 (2010).
124. *Diederik Vanfleteren*, Dimitri Van Neck, Patrick Bultinck, Paul W. Ayers, and Michel Warquier, "Partitioning of the Molecular Density Matrix Over Atoms and Bond," *Journal of Chemical Physics* **132**, 164111 (pp. 1-10) (2010).

Accepted Journal Articles

125. Steven Burger and Paul W. Ayers, "Methods for finding transition states on reduced potential energy surfaces", *Journal of Chemical Physics* (accepted).
126. Rogelio Cuevas-Saavedra and Paul W. Ayers, "Exchange-Correlation Functionals from the Identical-Particle Ornstein-Zernike Equation: Basic Formulation and Numerical Algorithms" *Int. J Modern Phys. B* (accepted) [invited article].
127. Steven Burger and Paul W. Ayers, "Quasi-Newton Parallel Geometry Optimization Methods", *Journal of Chemical Physics* (accepted).
128. James S. M. Anderson, Paul W. Ayers, and Juan I. Rodriguez-Hernandez, "How Ambiguous Is the Local Kinetic Energy", *J. Phys. Chem. A* (accepted) [invited article].

Submitted Journal Articles:

129. Paul W. Ayers and Mel Levy, "Time-Independent Density-Functional Theory for Excited States of Coulomb Systems"; *Physical Review Letters* (submitted).
130. Y. L. Liu and P. W. Ayers, "Finding Minimum Energy Reaction Paths on *Ab Initio* Potential Energy Surfaces Using the Fast-Marching Method", *Chem. Phys. Lett.* (submitted).
131. Paul W. Ayers and Samantha Jenkins, "Bond Metallicity Measures," *Phys. Chem. Chem. Phys.* (submitted).
132. Debajit Chakraborty and Paul W. Ayers, "Failure of the Weisacker Kinetic Energy Functionals for Higher-Order Electron Distribution Functions", *Theor. Chem. Acc.* (submitted).

133. Paul W. Ayers, "Energy Is Not a Convex Function of Particle Number for r^{-k} Interparticle Potentials with $k > 1.262$ ", *Phys. Rev. A, Rapid Communication* (submitted).
134. Steven K. Burger, David C. Thompson, and Paul W. Ayers, "QM/MM strategies for docking pose refinement: distinguishing between binders and decoys in cytochrome c peroxidase", *J. Phys. Chem. B* (submitted).
135. Steven K. Burger and Paul W. Ayers, "Empirical Prediction of Protein pKa Values With Residue Mutation", *Proteins* (submitted).

In Preparation (only papers with complete drafts available are included; these drafts are in the "iteration to convergence" stage):

136. James S. M. Anderson and Paul W. Ayers, "A Look at Relativistic Corrections to Atoms in Molecules" (in preparation for *J. Chem. Phys.*).
137. Rogelio Cuevas and Paul W. Ayers, "Legendre Transform Approach to the Scaling Properties of the Non-interacting Kinetic Energy and Exchange Functionals," (in preparation for *Chem. Phys. Lett.*).
138. Paul W. Ayers and Mel Levy, "A Tight Constraint on the Exchange-Correlation Potential Difference in Degenerate States", (in preparation for *Phys. Rev. A*).
139. Carlos Cardenas, Andres Cedillo, and Paul W. Ayers, "Reactivity Indicators for Degenerate States in the Density-Functional Theoretic Chemical Reactivity Theory", (in preparation for *J. Chem. Phys.*).
140. Carlos Cardenas, Frank De Proft, David Tozer, Paul Geerlings, and Paul W. Ayers, "Should Negative Electron Affinities Be Used For Evaluating the Chemical Hardness?", (in preparation for *J. Phys. Chem. A*).
141. Debajit Chakraborty, Carlos Cárdenas, Eleonora Echegaray, Paul W. Ayers, and Alejandro Toro-Labbe, "Understanding the Formation and Fracture of Chemical Bonds with the Reaction Force Profile and the Berlin Binding Function," (in preparation for *J. Phys. Chem. A*).
142. Rogelio Cuevas and Paul W. Ayers, "Alternative Ornstein-Zernike Models for the Exchange-Correlation Hole", (in preparation for *Phys. Rev. A*).

2.2 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 Théorique; Centre Nationale de la Recherche 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. Pacificchem (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 (confirmed, July 2006) [Girona]
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 Química; 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. Chinese Academy of Sciences, Shanghai Institute for Organic Chemistry; “overview” of computational chemistry” (November 2008) [China]
70. Laboratoire de Chimie Théorique; Centre Nationale de la Recherche Scientifique; (Dec. 2008) [France]
71. Department of Chemistry; University of Andres Bello (January, 2009) [Chile]
72. Department of Chemistry, York University (February 2009) [Canada]
73. Department of Chemistry, Queen’s University (February 2009) [Canada]
74. 2009 Molecular Informatics and Bioinformatics Symposium (March 2009) [Hungary]
75. Girona Workshop on Theoretical Chemistry (July 2009) [Spain]
76. Seventh Canadian Computational Chemistry Conference (July 2009) [Canada]
77. Fields Institute Workshop on Quantum Marginals and Density Matrices (July 2009) [Canada]
78. 33rd International Workshop on Condensed Matter Theories (August 2009) [Ecuador]
79. Department of Chemistry, Wayne State University (November, 2009) [U.S.A.]
80. Symposium “Of Molecules and Materials; A Survey of Recent Concepts” at Indian Institute for Scientific Education and Research (December, 2009) [India]
81. Symposium in the Theoretical Sciences, IIT-Kharagpur (December, 2009) [India]
82. Center for Theoretical Science, IIT-Kharagpur (January 2010) [India]
83. Indian Association for the Cultivation of Science, (January 2010) [India]
84. Department of Chemistry, Calcutta University, (January 2010) [India]
85. Symposium on Quantum Chemistry, Pontificia Universidad Católica de Chile [Chile]
86. Sanibel Symposium (February 2010, confirmed) [U.S.A.]
87. Department of Chemistry, Duke University (theoretical chemistry seminar) [U.S.A.]
88. Department of Chemistry, New York University (April 2010) [U.S.A.]
89. Brookhaven National Laboratory (April 2010) [U.S.A.]

90. FANTOM Study Week, Ghent University; Lecture Series with Two Talks (May 2010) [Belgium]
91. Canadian Society for Chemistry Conference (May 2010) [Canada]
92. 20th Birthday Conference for the Electron Localization Function (June 2010, confirmed) [France]
93. Gordon Conference, "Electron Densities and Chemical Bonding" (July 2010, confirmed) [U.S.A.]
94. 9th Girona Seminar, "Electron Density, Density Matrices, and Density-Functional Theory" (July 2010, confirmed) [Spain]
95. "Challenges in Density Functional Theory" at American Chemical Society National Meeting (August 2010, confirmed) [U.S.A.]
96. Girona Workshop on Theoretical Chemistry (October 2010, confirmed) [Spain]
97. Pacificchem (December 2010, confirmed) [U.S.A.]
98. Pacificchem (December 2010, confirmed) [U.S.A.]
99. 9th Conference of the World Association of Theoretically Oriented Chemists (July 2011, confirmed) [Spain]
100. American Chemical Society National Meeting (August 2011, confirmed) [U.S.A.]

2.3 Contributed Talks:

233rd National Meeting of the American Chemical Society (March 2007) [U.S.A.]

2.4 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]

2.5 Public Lectures:

Lecture on "Science in Society" at Highland Secondary School in Dundas (May, 2003).

2.6 Talks/Posters by Supervisees:

Graduate Student Symposium at the University of Buffalo; Univ. of Buffalo, United States (James Anderson; May 2005) [poster] [U.S.A.]

Graduate Student Symposium at the University of Buffalo; Univ. of Buffalo, United States (Juan Rodriguez; May 2005) [poster] [U.S.A.]

Recent Developments in Electronic Structure; Cornell Univ., United States (James Anderson; June 2005) [poster] [U.S.A.]

Simulation of Rare Events, The Reaction-Path Problem in Complex Systems; CECAM, France (Bijoy Dey; June 2005) [poster] [France]

Nanoscience at the Interface of Chemistry and Biology, Cancun, Mexico (Juan Rodriguez; August 2005) [talk] [Mexico]

Graduate Student Symposium at the University of Buffalo; Univ. of Buffalo, United States (James Anderson; May 2006) [talk] [U.S.A.]

EMBO Course/Conference on "Proteins: Structure, Dynamics, and Energetics" at the Shanghai Institute for Biological Sciences; Shanghai, China. (Annie Liu; May 2006) [poster]. [China]

6th European Conference on Computational Chemistry (Juan Rodriguez, August 2006) [poster]. [Slovakia]

Graduate School of Physics; Instituto Politecnico Nacional de Mexico (IPN) (Juan Rodriguez, December 2006) [invited talk] [Mexico]

234th National Meeting of the American Chemical Society. (James Anderson, August 2007) [talk] [U.S.A.]

234th National Meeting of the American Chemical Society. (James Anderson, August 2007) [poster] [U.S.A.]

234th National Meeting of the American Chemical Society. (Juan Rodriguez, August 2007) [poster] [U.S.A.]

235th National Meeting of the American Chemical Society. (Ivan Vinogradov, April 2008) [poster] [U.S.A.]

Women in Science and Engineering Conference (Annie Liu, April 2008) [talk] [Canada]

Canadian Chemistry Society Conference (Annie Liu, May 2008) [talk] [Canada]

Canadian Chemistry Society Conference (James Anderson, May 2008) [talk] [Canada]

Canadian Chemistry Society Conference (Ivan Vinogradov, May 2008) [talk] [Canada]

Canadian Chemistry Society Conference (Rogelio Cuevas, May 2008) [talk] [Canada]

Odyssey 2008, Mathematical and Computational Aspects of Molecular Electronic Structure Calculations (James Anderson, June 2008) [talk] [Canada]

Odyssey 2008, Mathematical and Computational Aspects of Molecular Electronic Structure Calculations (Rogelio Cuevas, June 2008) [talk] [Canada]

NSERC-USRA Undergraduate Student Poster Competition (Sandra Rabi, January 2009) [poster] [Canada]

Universidad de Guanajuato (Carlos Cardenas, January 2009) [invited talk] [Mexico]

Dept. of Physics; Higher School of Physics and Mathematics of the National Polytechnic Institute (Rogelio Cuevas, February 2009) [invited talk] [Mexico]

Southern Ontario Undergraduate Chemistry Conference (Sandra Rabi; March 2009) [talk] [Canada]

Women in Science and Engineering Conference (Nataly Rabi; March 2009) [poster] [Canada]

Center for Research in Molecular Modeling (Debajit Chakraborty; May 2009) [poster] [Canada]

New York Graduate Student Symposium at the Univ. of Buffalo (James Anderson; May 2009) [talk] [U.S.A.]

New York Graduate Student Symposium at the Univ. of Buffalo (Rogelio Cuevas; May 2009) [talk] [U.S.A.]

Canadian Society for Chemistry Conference (Sandra Rabi, June 2009) [poster] [Canada]

Canadian Society for Chemistry Conference (Carlos Cardenas, June 2009) [poster] [Canada]

Canadian Society for Chemistry Conference (Nataly Rabi, June 2009) [poster] [Canada]

Canadian Society for Chemistry Conference (Debajit Chakraborty, June 2009) [poster] [Canada]

Canadian Society for Chemistry Conference (Rogelio Cuevas, June 2009) [invited talk] [Canada]

Canadian Society for Chemistry Conference (James Anderson, June 2009) [invited talk] [Canada]

Canadian Society for Chemistry Conference (Steven Burger, June 2009) [talk] [Canada]

Canadian Society for Chemistry Conference (Eleonora Echegaray, June 2009) [talk] [Canada]

Canadian Society for Chemistry Conference (Paul Johnson, June 2009) [talk] [Canada]

Fields Institute Workshop on Quantum Marginals and Density Matrices (Paul Johnson, July 2009) [Canada]

Fields Institute Workshop on Quantum Marginals and Density Matrices (Carlos Cardenas, July 2009) [Canada]

Fields Institute Workshop on Quantum Marginals and Density Matrices (Rogelio Cuevas, July 2009) [Canada]

Fields Institute Workshop on Quantum Marginals and Density Matrices (Pavel Kulikov, July 2009) [Canada]

Fields Institute Workshop on Quantum Marginals and Density Matrices (James Anderson, July 2009) [Canada]

Seventh Canadian Computational Chemistry Conference (Rogelio Cuevas, July 2009) [poster] [Canada]

Seventh Canadian Computational Chemistry Conference (Ivan Vinogradov, July 2009) [poster] [Canada]

Seventh Canadian Computational Chemistry Conference (Carlos Cardenas, July 2009) [poster] [Canada]

Seventh Canadian Computational Chemistry Conference (Eleonora Echegaray, July 2009) [poster] [Canada]

DFT2009; 13th International Conference on the Theory and Applications of Density Functional Theory (Carlos Cardenas, August 2009) [poster] [France]

Theoretical Chemistry Group, Beijing University (James Anderson, October 2009) [invited talk] [China]

Department of Chemistry; Vrije Universiteit Brussels (Carlos Cardenas, Oct. 2009) [invited talk] [Belgium]

Departments of Chem. and Phys.; UAM-Iztapalapa (Carlos Cardenas, Nov. 2009) [invited talk] [Mexico]
 Waterloo Chemical Physics Conference (Paul Johnson, November 2009) [poster] [Canada]
 Waterloo Chemical Physics Conference (Debajit Chakraborty, November 2009) [poster] [Canada]
 Waterloo Chemical Physics Conference (Helen Van Aggelen, November 2009) [poster] [Canada]
 Waterloo Chemical Physics Conference (Steven Burger, November 2009) [talk] [Canada]
 Waterloo Chemical Physics Conference (Rogelio Cuevas, November 2009) [talk] [Canada]
 41st Inorganic Discussion Weekend (Paul Johnson, November 2009) [talk] [Canada]
 Undergraduate Student Research Award Poster Session (Paul Johnson, November 2009) [poster] [Canada]
 Department of Chemistry, Univ. Andres Bello (Carlos Cardenas, December 2009) [invited talk] [Chile]
 Department of Chemistry, Wayne State University (Steven Burger, April 2010) [invited talk] [Canada]
 Women in Science and Engineering Conference (Sandra Rabi; March 2010) [talk] [Canada]
 Graduate Student Symposium at the University of Buffalo; Univ. of Buffalo, United States (James Anderson;
 May 2010) [talk] [U.S.A.]
 Graduate Student Symposium at the University of Buffalo; Univ. of Buffalo, United States (Paul Johnson;
 May 2010) [talk] [U.S.A.]
 Canadian Society for Chemistry Conference (Steven Burger, June 2010) [talk] [Canada]
 Canadian Society for Chemistry Conference (Nataly Rabi, June 2010) [poster] [Canada]
 Canadian Society for Chemistry Conference (Rogelio Cuevas, June 2010) [poster] [Canada]
 Canadian Society for Chemistry Conference (Rogelio Cuevas, June 2010) [poster] [Canada]
 Canadian Society for Chemistry Conference (Paul Johnson, June 2010) [poster] [Canada]
 Canadian Society for Chemistry Conference (Paul Johnson, June 2010) [poster] [Canada]
 Canadian Society for Chemistry Conference (Eleonora Echegaray, June 2010) [poster] [Canada]
 Canadian Society for Chemistry Conference (Debajit Chakraborty, June 2010) [poster] [Canada]
 Canadian Society for Chemistry Conference (Ahmed Mohammed, June 2010) [poster] [Canada]
 Canadian Society for Chemistry Conference (James Anderson, June 2010) [poster] [Canada]

3. Leadership

3.1 Reviewing, Refereeing, and Adjudicating

3.1.a Journals [368 reviews for 47 different journals and 3 different books (since 2003)]

ACM Transactions on Mathematical Software (1); Advances in Quantum Chemistry (1); African Journal of Pure and Applied Chemistry (1); Biophysical Chemistry (6); Canadian Journal of Chemical Engineering (1); Canadian Journal of Chemistry (2); Chemistry, a European Journal (4); Chemical Physics (2); Chemical Physics Letters (23); Collection of Czechoslovak Chemical Communications (1); Coordination Chemistry Reviews (1); Crystal Growth and Design (3); Dalton Transactions (3); European Journal of Chemistry (2); European Journal of Inorganic Chemistry (1); European Journal of Physics D (1); Inorganic Chemistry (10); International Journal of Chemical Kinetics (1); International Journal of Quantum Chemistry (24); Journal of the American Chemical Society (2); Journal of Chemical Physics (66); Journal of Chemical Sciences (2); Journal of Chemical Theory and Computation (16); Journal of Computational Chemistry (14); Journal of Mathematical Chemistry (2); Journal of Organic Chemistry (7); Journal of Physical Chemistry (40); Journal of Physical Organic Chemistry (2); Journal of Physics A (Mathematical and General) (5); Journal of Physics B (Condensed Matter) (6); Journal of Physics and Chemistry of Solids (1); Journal of Theoretical and Computational Chemistry (5); Macromolecules (1); Molecular Physics (5); New Journal of Chemistry (1); Organic Letters (1); Pharmaceutical Research (1); Physica B (2); Physical Biology (1); Physical Chemistry Chemical Physics (14); Physics Letters A (2); Physical Review A (9); Physical Review B (15); Physical Review E (1); Physical Review Letters (23); Research Letters in Physical Chemistry (1); THEOCHEM, Journal of Molecular Structure (13); Theoretical Chemistry Accounts (9)

I serve as an adjudicator for the *Journal of Chemical Physics*, *Journal of Physical Chemistry A*, *Journal of Physics B*, *Physical Review A*, *Physical Review B*, and *Physical Review Letters*.

3.1.b Grants (0)

CIHR (1); Fondecyt-Chile (1); NSERC (12); NSF (5); NSF Career Award (2); Research Corporation (3); SHARCNET Research Fellowship (5); Hasselt University (Belgium) Funding Award (1); Research Grants Council, Hong Kong (1)

3.1.c External Referee for Tenure Decision [St. Mary's University (Canada); Nanyang Technological University (Singapore)]

3.1.d Member of the Editorial Board: THEOCHEM, Journal of Molecular Structure, 2009-present

3.1.e Member of the delegation from the Canadian Society for Chemistry to China, 2008

3.2 Conference Organizer

231st National Meeting of the American Chemical Society National Meeting "Frontier Applications and Developments of Density Functional Theory" (March 2006; Computational/Physical Divisions; co-organizer with W. Yang)

92nd Canadian Chemistry Conference and Exhibition, "Atoms in Molecules" (May 2009; co-organizer with Cherif Matta)

92nd Canadian Chemistry Conference and Exhibition, "Static Electron Correlation" (May 2009; co-organizer with Marcel Nooijen)

3.3 Conference Session Chair:

16th Canadian Symposium on Theoretical Chemistry (August, 2007) [Canada]

92nd Canadian Chemistry Conference and Exhibition (May, 2009) [2 sessions; Canada]

60th Birthday Symposium for Swapan Ghosh; Center for Theoretical Science, IIT-Kharagpur [India]

Twenty Years of the Electron Localization Function; CNRS, Paris [France]

3.4 Recognized Publications [updated yearly in January]

Coauthor of #1 Most Accessed Paper in *Journal of Physical Chemistry A* (2005). [The same paper was #1 most accessed in the Jan-Jun 2005 and Oct-Dec. 2005 time periods. It was #17 in the intervening time period. From Jan.-Mar. 2006 this was the most accessed article in the "Molecular Structure, Bonding, Quantum Chemistry, and General Theory" section of this journal; from April-June 2006 it was #2 in this section. [Two years after the initial publication (Jan-Mar, 2007) it was *still* the #15 most accessed paper in JPCA (every other paper on the list is from 2007!)]

Coauthor of Highly Accessed Paper in *Journal of Chemical Theory of Computation* (#11 Jan-Mar. 2007; #9 Apr-June 2007; #14 for the entire year).

Author of #2 Most Downloaded Paper in *Faraday Discussions* (Jan, 2007). [The same article was #3 in Feb., 2007, #7 in March and April, 2007, and #10 in May, 2007.]

Author of #8 Most Downloaded Paper in *Molecular Physics* from 2006.

Publication #76 was flagged as a "very important paper" and featured in *Chemistry, A European Journal*.

Publication #80 was the 10th most accessed paper in *J. Phys. Chem. A* from Oct.-Dec. 2007.

Publication #54 was the 4th most downloaded paper from *J. Chem. Phys.* in Dec., 2006.

Publication #67 was the 12th most downloaded paper from *J. Chem. Phys.* in April, 2007.

Publication #106 was the 3rd most downloaded paper from *J. Chem. Phys.* in July, 2009.

Publication #4 is the 2nd most cited paper in *Theor. Chem. Acc.* in 2000.

Publication #7 is in the 5% most cited articles in *J. Am. Chem. Soc.* in 2000.

Publication #11 is the 10th most cited article in *Theor. Chem. Acc.* in 2001.

Publication #16 is the 10th most cited article in *Int. J. Quantum Chem.* in 2002.

Publication #27 is the 2nd most cited article in *Int. J. Quantum Chem.* in 2005.

Publication #29 is the 20th most cited article in *Phys. Chem. Chem. Phys.* in 2005

Publication #30 is the 3rd most cited article in *J. Math. Phys.* in 2005.

Publication #31 is the 8th most cited article in *J. Phys. Chem. A* in 2005.

Publication #37 is the 6th most cited article in *J. Chem. Sci.* in 2005.
Publication #39 is the most cited article in *J. Chem. Sci.* in 2005.
Publication #44 is in the 5% most cited articles in *J. Chem. Phys.* in 2006.
Publication #48 is in the 2% most cited articles in *J. Chem. Phys.* in 2006.
Publication #56 is the most cited article in *Faraday Discussions* in 2007.
Publication #63 is the 15th most cited article in *J. Chem. Theory Comp.* in 2007
Publication #71 is the 4th most cited article in *Adv. Chem. Phys.* in 2007.
Publication #81 is the most cited article in *J. Math. Chem.* in 2008.
Publication #84 is in the 5% most cited articles in *J. Chem. Phys.* in 2008.
Publication #96 is the 8th most cited article in *J. Math. Chem.* from 2009.
Through 2008, on average, my articles are in the top quartile of articles from their respective journals in terms of citations.

3.5 International Exchanges

I have visited the following universities for extended (typically month-long) periods:

- UAM-Itzapalapa (Mexico; 2003)
- Vrije Universiteit Brussel (Belgium; 2004, 2007)
- Univ. of Ghent (Belgium; 2005, 2008 (twice), 2009 (twice))
- Inst. of Theoretical Physics; Univ. of Debrecen (Hungary; 2006)
- Nucleus for Applied Quantum Mech. and Computational Chem. (Santiago, Chile; 2007, 2008, 2009, 2010)
- CNRS, Paris (France, 2008, 2009)
- Universidad de Guanajuato (Mexico, 2008)
- Beijing University (China, 2008)

The following senior scientists have visited McMaster for extended stays:

- Andres Cedillo (UAM-Itzapalapa, Mexico; 2005)
- Junia Melin (Kansas State University, U.S.A.; 2005, 2009)
- Samantha Jenkins (University West, Sweden; 2008, 2009)
- Steven Kirk (University West, Sweden; 2008, 2009)

3.6 International Consortium

I am a foreign member of the Scientific Research Network “Quantum Chemistry : fundamental and applied Aspects of Density Functional Theory” funded by the *Research Foundation, Flanders (FWO-Vlaanderen)*.

4. Training

High-School Co-op Students:

Sung-Min Lee (1/2007-8/2007)

Undergraduates Thesis Students:

- Stuart Bothwell (10/2003-4/2004)
- Sarah Rauscher (10/2003-4/2004)
- Allison Chapman (10/2004-4/2005)
- Karl Jobst (9/2005-4/2006) [co-supervised with Prof. Hans Terlouw]
- Mathew Komorowski (9/2006-6/2007)
- Sandra Rabi (9/2008-4/2009)
- Nataly Rabi (9/2010-4/2011)
- Ankit Rastogi (9/2010-4/2011)
- Michael Lacasse (9/2020-4/2011)

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.)
David Kim (5/2010-8/2010; Chemistry, McMaster Univ.)
Melissa Ng (6/2004-12/2004; Mathematics, McMaster Univ.)
Nataly Rabi (5/2008-8/2010; Chemistry, McMaster Univ.)
Sandra Rabi (5/2006-8/2008; Chemistry, McMaster University)
Santa Rabi (5/2010-8/2010; Health Science, McMaster University)
Sarah Mansour (Rauscher) (5/2004-8/2004; Physics, McMaster Univ.)
Jordan Thomson (5/2004-8/2004; 5/2005-8/2005; Chemistry, McMaster Univ.)
Marie Yan (5/2010-8/2010; Health Sciences; McMaster Univ.)

Graduate Students:

James S. M. Anderson (2004-present)
Debajit Chakraborty (2007-present)
Rogelio Cuevas (2007-present)
Eleonora Echegaray (2008-present) [joint with Alejandro Toro Labbe; PUC, Chile]
Paul Johnson (2009-present)
Ahmed Mohammed (2009-present)
Pavel Kulikov (2008-present)
Yuli (Annie) Liu (2004-present)
Sandra Rabi (2009-present)
Juan I. Rodriguez Hernandez (2003-2008)
Ivan Vinogradov (2005-present)

Post-Doctoral Research Associates:

Steven Burger (9/2007 - present)
Carlos Cardenas (4/2008-4/2010)
Alfredo Guevara (5/2009-6/2010)
Bijoy K. Dey (8/2003-3/2005;10/2005-2/2007)
Lourdes Romero (5/2008 – 5/2009)
Utpal Sarkar (4/2006-6/2007)
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 am the advisor to the chapter) (2009)

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) (2009) [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)
1st year student research fellowship (David Kim) (2010)
Health Sciences Undergraduate Research Award (Santa Rabi) (2010)