Jaime M. Martell

Cape Breton University Sydney, Nova Scotia B1P 6L2 (902) 562-0812 (H); (902) 563-1211 (W)

E-Mail: jaime_martell@cbu.ca Web: http://faculty.cbu.ca/jmartell

EDUCATION

1991-95	Dalhousie University Halifax, Nova Scotia Thesis: <i>Ab Initio</i> Studies of Fluorinate Properties and Reactions with Hydro Supervisor: Dr. Russell J. Boyd External Examiner: Dr. Kenneth B. V	xyl Radicals
1987-91	St. Mary's University Halifax, Nova Scotia Thesis: Rydberg Series in the Arc Spo Supervisor: Dr. William E. Jones	B.Sc. (Honours) Chemistry ectrum of Antimony
1981-82	Nova Scotia College of Geographic Sciences Lawrencetown, Nova Scotia	Dip.T. Scientific Computer Programming
1978-80	University College of Cape Breton Sydney, Nova Scotia	Dip.T. Chemical Technology
ACADEMIC POSITIONS		
2008 -	Cape Breton University	Associate Professor
2004-08	Cape Breton University	Assistant Professor
2003-04	Acadia University	Assistant Professor
1999-2003	SUNY Potsdam	Assistant Professor
1997-99	Lyon College/ UNC Asheville	Camille and Henry Dreyfus Fellow
1995-97	University of Guelph	Postdoctoral Fellow

TEACHING EXPERIENCE

Sept. – Dec. (2005, '07, '09)	General Chemistry I, Cape Breton University
Jan Apr. (2006, 2010)	General Chemistry II, Cape Breton University
Jan. – Apr. (2005, '07) Sept. – Dec. 2008	Advanced Physical Chemistry, Cape Breton University
Jan Apr. (2005-10)	Chemical Kinetics and Equilibrium, Cape Breton University
Sept. – Dec. (2004, '06)	Intermediate Physical Chemistry, Cape Breton University
Sept. – Dec. (2004, '06-09)	Chemical Thermodynamics, Cape Breton University
Sept. 2003 – Apr. 2004	Introductory Chemistry for the Physical Sciences, Acadia University
Jan Apr. 2004	Physical Chemistry 3 (Quantum Chemistry), Acadia University
Sept. – Dec. 2003	Structure and Bonding, Acadia University
Aug. 1999 – May 2003	Physical Chemistry lectures and labs, SUNY Potsdam
Aug. 2000 – Dec. 2002	Fundamentals of Environmental Science (non-majors course), SUNY Potsdam
Aug. 1999 – May 2000	General Chemistry labs, SUNY Potsdam
Aug. 1998 - May 1999	General Chemistry labs, University of North Carolina at Asheville
Aug. 1997 - May 1998	Physical Chemistry labs, team teaching Physical Chemistry lectures, Lyon College
Sept Dec., 1996	Lecturer, Chemistry Today, University of Guelph

(Also significant teaching assistant experience, graduate and undergraduate; included TAing labs and grading assignments, for Physical, General, and Organic Chemistry courses)

RESEARCH EXPERIENCE**

Aug. 2004 - present	Cape Breton University	Assistant/Associate Professor
present	Theoretical studies of unimolecular eliminate substituted formaldehydes, and hydrohaloeth of potential anti-tumour drugs and vitamins.	•
Aug. 1999 - June 2003	SUNY Potsdam	Assistant Professor
June 2003	Theoretical studies of unimolecular eliminate substituted formaldehydes; modelling of alky	
Aug. 1997 - Aug. 1999	Lyon College/UNC Asheville	Dreyfus Postdoctoral Fellow
rug. 1777	Theoretical studies of substituent effects for reactions of gas-phase haloalkanes and haloa	
June 1996	Stockholm University	Visiting Scientist
	Computational investigation of hyperfine str	uctures of some sulfur oxides.
Sept. 1995 - Aug. 1997	University of Guelph	Postdoctoral Researcher
Aug. 1997	Computational investigations of reactions of calibration of Density Functional Theory me assist in supervision of graduate students; de	thods for reaction energetics;
July - Aug. 1995	Saint Mary's University	Postdoctoral Researcher
	Calculation of stacking interactions, training of students in computational chemistry techniques, system administration.	
June 1995	Dalhousie University	Postdoctoral Researcher
	Topological analyses of reactions.	
Summer 1990	Saint Mary's University	NSERC Summer Student
	Laser chemistry and surface study experimen	nts.

^{*} Also see theses on page 1.

Summer 1989	Saint Mary's University	NSERC Summer Student
	Organometallic synthesis.	
1984 - 89	Bedford Institute of Oceanography Dartmouth, Nova Scotia	Computer Programmer/ Data Processor
	Software development and maintenance, user su analysis and production of plots, compilation of of physical oceanography research projects.	- -
Nov. 1982 - Apr. 1983	Martec Ltd. Halifax, Nova Scotia	Computer Programmer
	Software development and data processing for s Gulf of St. Lawrence.	tudy of ice conditions in
July - Oct. 1980	Technical University of Nova Scotia Halifax, Nova Scotia	Research Assistant
	Assisted supervisor in setting up a solid fuel contesting laboratory, performed test and wrote repowood stove.	

PUBLISHED RESEARCH

JOURNAL PUBLICATIONS

Meghan M. MacIntyre*, Jaime M. Martell, and Leif A. Eriksson, "DFT study of five naphthalimide derivatives: Structures and redox properties", *Theochem*, **2010**, *941*, 133-137.

Jaime M. Martell, Paul T. Beaton*, and Bert E. Holmes, "Comparisons between Density Functional Theory and Conventional *ab initio* Methods for 1,2-Elimination of HF From 1,1,1-Trifluoroethane: Test Case Study for HF Elimination From Fluoroalkanes", *J. Phys. Chem. A*, **2002**, *106*, 8471 - 8478.

Maria O. Burgin*, George L. Heard, Jaime M. Martell, and Bert E. Holmes, "Unimolecular Reaction Kinetics of CF₂ClCF₂CH₃ and CF₂ClCF₂CD₃: Experimental Evidence for a Novel 1,2-FCl Rearrangement Pathway", *J. Phys. Chem. A* **2001**, *105*, 1615-1621.

^{* =} undergraduate research student

Jaime M. Martell, Hengtai Yu and John D. Goddard, "Molecular Decompositions of Acetaldehyde and Formamide: Theoretical Studies Using Hartree-Fock, Møller-Plesset and Density Functional Theories", *Mol. Phys.* **1997**, *92*, 497-502.

Jaime M. Martell, Leif A. Eriksson and John D. Goddard, "Assessment of Basis Set and Functional Dependencies in Density Functional Theory: Studies of Atomization and Reaction Energies", *J. Phys. Chem.* A **1997**, *101*, 1927-1934.

Jaime M. Martell, Leif A. Eriksson, and John D. Goddard, "A Density Functional Study of the Hyperfine Properties of Sulfur Containing Radicals and Radical Ions", *Acta Chem. Scand.* **1997**, *51*, 229-232.

Jaime M. Martell, James B. Tee* and Russell J. Boyd, "Topological Properties of the Reactants, Transition States, and Products of the Hydroxyl Radical with the Series $C_2H_nF_{6-n}$, n=1-6", *Can. J. Chem.* **1996**, *74*, 786-800.

Jaime M. Martell and Russell J. Boyd, "*Ab Initio* Studies of Reactions of Hydroxyl Radicals with Fluorinated Ethanes", *J. Phys. Chem.* **1995**, *99*, 13402-13411.

Jaime M. Martell, Anil K. Mehta*, Philip D. Pacey and Russell J. Boyd "Properties of Transition Species in the Reaction of Hydroxyl with Ethane from ab Initio Calculations and Fits to Experimental Data", *J. Phys. Chem.* **1995**, *99*, 8661-8668.

Jaime M. Martell, Russell J. Boyd and Leif A. Eriksson, "Hyperfine Structures of the Series $C_2H_nF_{5-n}$, n=0-5: A Density Functional Theory Study", *J. Phys. Chem.* **1995**, *99*, 623-629.

Jaime M. Martell, Russell J. Boyd and Zheng Shi, "Effects of Electron Correlation on the Series $C_2H_nF_{6-n}$ (n = 0-6): Geometries, Total Energies and C-C and C-H Bond Dissociation Energies", *J. Phys. Chem.* **1993**, *97*, 7208-7215.

Jaime M. Martell and Russell J. Boyd, "Ab Initio Studies of the Series $C_2H_nF_{6-n}$ (n = 0-6): Geometries, Total Energies and C-C Bond Dissociation Energies", J. Phys. Chem. **1992**, 96, 6287-6290.

William E. Jones and Jaime M. Martell*, "Rydberg Series in the Arc Spectrum of Antimony", *Can. J. Phys.* **1991**, *69*, 891-896.

Jaime M. Martell* and Michael J. Zaworotko, "Synthesis and Structure of Mixed Chloride-Tetrachloroaluminate Salts", *J. Chem. Soc. Dalton Trans.* **1991**, 1495-1498.

HONOURS THESES SUPERVISED

Alex Lee, "The Ability of DFT Functionals PBE1PBE and BMK to Predict Atomization Energies and Enthalpies of Formation", 2009

Curtis W. White, "Hydrogen Abstraction from Fluorinated Ethyl Methyl Ether Systems by OH Radicals", 2007/08.

Meghan M. MacIntyre, "Computational study of the use of naphthalimide derivatives as photosensitizers for selective oxidation of guanine in DNA", 2006/07.

CONFERENCE PRESENTATIONS

Qi Xu and <u>Jaime Martell</u>, "Computational Study of the Photodecomposition of Pyridoxine", 12th Atlantic Theoretical Chemistry Symposium, August, 2011, Charlottetown, PEI.

<u>Jaime Martell</u>, Matthias Bierenstiel, and C. Dale Keefe, "Chemical Education Initiatives at Cape Breton University", Maritimes CIC Section Annual General Conference and Meeting, June 2011, Moncton, NB.

<u>Jaime M. Martell</u>, "Trials, Tribulations and Tribulations of Optimizing Transition States", 10th Atlantic Theoretical Chemistry Symposium, July, 2009, Fredericton, NB.

<u>W. Cory McNeil*</u> and Jaime M. Martell, "Short Chain Alcohols - Investigation of 1,2 HOH Elimination Pathways", 9th Atlantic Theoretical Chemistry Symposium, August, 2008, Sydney, NS.

<u>Curtis W. White*</u> and Jaime M. Martell, "Hydrogen Abstraction from Fluorinated Ethyl Methyl Ether Systems by OH Radicals", 9th Atlantic Theoretical Chemistry Symposium, August, 2008, Sydney, NS.

<u>Colin Andrews*</u> and Jaime M. Martell, "AIM Analyses of Transition States for Hydrogen Abstraction from Fluorinated Ethers", 9th Atlantic Theoretical Chemistry Symposium, August, 2008, Sydney, NS.

<u>Cara Andrews*</u> and Jaime M. Martell, "DFT Studies of Halogenated Propenes and Butenes", 9th Atlantic Theoretical Chemistry Symposium, August, 2008, Sydney, NS.

Curtis W. White* and <u>Jaime M. Martell</u>, "Hydrogen Abstraction from Fluorinated Ethyl Methyl Ether Systems by OH Radicals", 91st Canadian Chemistry Conference and Exhibition, May 2008, Edmonton, AB.

<u>Jaime M. Martell</u>, Meghan M. MacIntyre* and Leif A. Eriksson, "Computational study of the use of naphthalimide derivatives as photosensitizers for selective oxidation of guanine in DNA", 16th Canadian Symposium on Theoretical Chemistry, August, 2007, St. John's, NL.

<u>W. Cory McNeil*</u> and Jaime M. Martell, "Transition States For 1,2 Elimination Of HX From Halogenated Propanes", 8th Atlantic Theoretical Chemistry Symposium, August, 2007, St. John's, NL.

<u>Curtis W. White*</u> and Jaime M. Martell, "Unimolecular Decomposition Pathways of Halogenated Ethylmethyl Ethers: A Density Functional Theory Study", 8th Atlantic Theoretical Chemistry Symposium, August, 2007, St. John's, NL.

<u>Jaime M. Martell</u> and John D. Goddard, "Density Functional Theory and Atoms In Molecules Studies of the Molecular Decompositions of FCHO, ClCHO, and HOCHO", 7th Atlantic Theoretical Chemistry Symposium, August 2006, Antigonish, NS.

<u>W. Cory McNeil*</u> and Jaime M. Martell, "1,2 HOH Elimination Pathways for Short Chain Alcohols", 7th Atlantic Theoretical Chemistry Symposium, August 2006, Antigonish, NS.

<u>Jaime M. Martell</u>, "Unimolecular Decomposition Pathways of Hydrohaloethers: A Density Functional Theory Study", 89th Canadian Chemistry Conference and Exhibition, May 2006, Halifax, NS.

<u>Jaime M. Martell</u>, "Unimolecular Decomposition Pathways of Hydrohaloethers: Preliminary Density Functional Theory Results", 6th Atlantic Theoretical Chemistry Symposium, August 2005, Sackville, NB.

<u>Jaime M. Martell</u>, Carl J. LaShomb* and John D. Goddard, "Density Functional Theory Studies of the Molecular Decompositions of FCHO, ClCHO, and HOCHO", 14th Canadian Symposium on Theoretical Chemistry, August, 2001, Ottawa, Ontario.

Jaime M. Martell, Carl J. LaShomb* and <u>John D. Goddard</u>, "Density Functional Theory Studies of the Molecular Decompositions of FCHO, ClCHO, and HOCHO", Symposium in Honor of Professor Ernest R. Davidson, July 2001, Seattle, Washington (invited poster).

<u>Eric Sandvig*</u> and Jaime Martell, "Computational Studies of the Elimination of Water from Ethanol", Learning and Research Fair, SUNY Potsdam, March 30, 2000.

Peter Morgan*, Anthony Molinero and Jaime Martell, "Modeling Studies on the Asymmetric Alkylation of β-Keto Esters", Learning and Research Fair, SUNY Potsdam, March 30, 2000.

<u>Jaime M. Martell</u> and Bert E. Holmes, "Transition States for 1,2 Elimination of HX (X = F, Cl) From Trifluoroethane and Chloroethane: Test Case Studies", 13th Canadian Symposium on Theoretical Chemistry, August, 1998, Vancouver, British Columbia.

<u>Jaime M. Martell</u> and Bert E. Holmes, "Transition States for 1,2 Elimination of HF from Fluoropropanes", 215th ACS National Meeting, March 1998, Dallas, Texas.

<u>Jaime M. Martell</u> and John D. Goddard, "Density Functional Theory Studies of the Molecular Decompositions of FCHO, ClCHO, and HOCHO", 7th International Congress of Quantum Chemistry, June, 1997, Atlanta, Georgia.

<u>John D. Goddard</u>, Xiao-Qing Chen and Jaime M. Martell, "Application of Density Functional Theory to Free Radical Structures and Energetics", 7th International Congress of Quantum Chemistry, June, 1997, Atlanta, Georgia (invited talk).

Wai-To Chan, <u>Jaime M. Martell</u>, John D. Goddard and Ian Hamilton, "An Atoms In Molecules Study of the Dimers of 1,2,3,5-dithiadiazolyl and 1,2,3,5-diselenadiazolyl radicals and Their Fluoro- and Methyl-Substituted Analogues", 80th Canadian Chemistry Conference and Exhibition, June, 1997, Windsor, Ont.

<u>Jaime M. Martell</u> and John D. Goddard, "Density Functional Theory Investigations of Molecular Decompositions of Substituted Formaldehydes: Geometries, Barrier Heights and Reaction Enthalpies", 80th Canadian Chemistry Conference and Exhibition, June, 1997, Windsor, Ont.

Wai-To Chan, <u>Jaime M. Martell</u>, John D. Goddard and Ian Hamilton, "An Atoms In Molecules study of the 1,2,3,5-dithiadiazolyl and 1,2,3,5-diselendiazolyl radicals", Symposium on the Occasion of the 65th Birthday of Richard F.W. Bader, October, 1996, Hamilton, Ont.

<u>Jaime M. Martell</u>, "A Study by Density Functional Theory of the Hyperfine Properties of Sulfur Containing Radicals and Radical Ions - A Problem Case", 14th International Conference on Radical Ions, July 1996, Uppsala, Sweden (invited poster).

<u>Jaime M. Martell</u> and Russell J. Boyd, "*Ab Initio* Studies of Reactions of Hydroxyl Radicals with Fluorinated Ethanes", 1995 Atlantic Student Chemistry Conference, May 1995, Halifax, N.S.

<u>Jaime M. Martell</u> and Russell J. Boyd, "Environmental Chemistry Meets the Information Highway: Computational Studies of CFC Alternatives", Symposium on Environmental Chemistry, October 1994, Halifax, N.S.

<u>Jaime M. Martell</u>, James B. Tee* and Russell J. Boyd, "Charge Development in the Transition States of the Reactions of Fluorinated Ethanes with Hydroxyl Radicals", International Conference on Radical Ions, August 1994, Halifax, N.S.

<u>Jaime M. Martell</u> and Russell J. Boyd, "*Ab Initio* Studies of the Reactions of OH With Fluorinated Ethanes", 2nd Canadian Computational Chemistry Conference, May 1994, Kingston, Ont.

<u>Jaime M. Martell</u>, Russell J. Boyd and Zheng Shi, "*Ab Initio* Studies of Fluorinated Ethanes: Properties and Reactions With Hydroxyl Radicals", Atlantic Division of Chemical Institute of Canada Conference, August 1993, Sydney, N.S.

<u>Jaime M. Martell</u>, Russell J. Boyd and Zheng Shi, "*Ab Initio* Studies of Fluorinated Ethanes", 76th Canadian Chemistry Conference and Exhibition, May 1993, Sherbrooke, P.Q.

<u>Jaime M. Martell</u>, "Trials and Tribulations of Optimizing Transition States: the Ethane + OH Reaction", 5th Atlantic Theoretical Chemistry Symposium, May 1993, Halifax, N.S.

SCHOLARSHIPS AND AWARDS

2003	President's Award for Excellence in Teaching, SUNY Potsdam (student nominated; not awarded)
1999	Camille and Henry Dreyfus Fellowship Supplemental Award (\$10,000), SUNY Potsdam
1998-99	Camille and Henry Dreyfus Fellowship, University of North Carolina at Asheville
1997-98	Camille and Henry Dreyfus Fellowship, Lyon College
1994-95	Walter C. Sumner Fellowship, Dalhousie University
1993-95	NSERC PGS B, Dalhousie University
May 1993	Co-winner, best student talk at 5 th Atlantic Theoretical Chemistry Symposium
1991-93	NSERC PGS 1&2, Dalhousie University
1991-95	Graduate Scholarship, Dalhousie University
1990-91	Charles Hinman Memorial Bursary, Saint Mary's University
1990-91	Achievement Scholarship, Saint Mary's University
1990	NSERC USRA, Saint Mary's University
1989-90	Dean's List, Saint Mary's University

Jaime Martell curriculum vitae

1989	NSERC USRA, Saint Mary's University
1979-80	Engineering Technology Scholarship, University College of Cape Breton
1978-80	Highest academic achievement in Chemical Technology program, University College of Cape Breton

GRANTS

CBU RP grant (summer 2010), "Computational Study of the Photodecomposition of Vitamin B3", \$6987.71.

CBU RP grant (summer 2010), "Computational Study of the Photodecomposition of Vitamin B6", \$6115.

CBU RP grant, (2008/09), "Computational Studies of Pathways of Some Atmospherically Significant Reactions"; \$1792.

NSERC Atlantic Regional Opportunities Fund (2008), "Seminar Tour for Dr. Stacey Wetmore", \$1614.

CBU RP grant, (summer 2008) "Computational Studies of Pathways of Some Atmospherically Significant Reactions"; \$5000.

CBU RP grant, (2007/08), "Computational Studies of Pathways of Some Atmospherically Significant Reactions"; \$2408.

CBU RP grant, (summer 2007) "Computational Studies of Pathways of Some Atmospherically Significant Reactions"; \$5000.

NSERC Discovery Grant, (2007-10) "Computational Studies of Reactions With Atmospheric Implications Using DFT and AIM Methodologies"; \$23,500 per annum for 3 years.

NSERC Research Tools and Instrumentation Grant, (2007) "Compute Nodes for a Linux Cluster for Computational Chemistry Research"; \$19,803.

CBU RP grant, (2006/07), "Computational Studies of Pathways of Some Atmospherically Significant Reactions"; \$3060.

SUNY Potsdam Curriculum Development Program, (2002-03) "Enhancing Data Analysis in Chemistry Laboratories Through the Use of a Professional Scientific Graphing Program", coauthored with David Gingrich; \$1000.

National Center for Supercomputing Applications Startup Award (07/00-06/01) "Density Functional Theory Studies on the Asymmetric Alkylation of β -Keto Esters"; 4000 SGI Origin 2000 hours.

SUNY Potsdam Mini-Grant, (1999-2000) "Computational Study of the Elimination of Water from Ethanol"; \$500.

North Carolina Supercomputing Center Campus Visualization Initiative (1999-2001) "Visualization and HPC as Tools for Undergraduate Research and Curriculum Enhancement"; Indefinite loan (minimum three years) of an SGI O2 workstation, visualization software (AVS and Unichem), training and support (approximate value \$25,000).

North Carolina Supercomputing Center Allocation Award (09/98-10/99) "Ab Initio Investigations of the Nature of Transition States for Unimolecular 1,1- and 1,2-Dehydrohalogenations of Haloalkanes"; 25 T90 Cray and 100 Cluster hours.

North Carolina Supercomputing Center Allocation Award (03/99-02/00) "*Unimolecular Kinetics of Haloalkanes, Haloalcohols and Haloethers*"; 245 T90 Cray and 5,620 SGI Origin hours.

UNIVERSITY SERVICE WORK SUNY Potsdam

Sept. 2000 – Aug. 2002	Chemistry department representative to Faculty Senate.
Oct. 2000 - Aug. 2002	Faculty Senate representative to Teaching and Learning with Technology Roundtable.
April 2001 - May 2003	Faculty advisor to Chemistry Club.
Aug. 2001 - May 2002	Member of faculty group designing new major in Environmental Studies
Oct. 2001 - May 2002	Advisory Council for Environmental Technician Program, St. Lawrence College, Cornwall, ON
Oct. 2001 - June 2002	At-large member of Arts & Sciences Council.

Cape Breton University

July 2006 – June 2008	Recording Secretary of School of Science and Technology
July 2006 – June 2007	Chemistry department representative to Academic Council
Sept. 2006 – June 2007	Teaching and Learning Committee
Sept. 2006 -	Chemistry Honours Thesis Committee
Jan. 2007 -	CBUFA Publicity Committee
Sept. 2007 – Aug. 2008	Research Committee of Senate
February 2008 – June 2009	Recording Secretary of Department of Chemistry
June 2008 -	Research Appeals Board
July 2008 – January 2010	Member-at-Large, CBUFA Executive
July 2008 - June 2009	Vice Chair of School of Science and Technology
Feb. 2009	Travel Policies and Procedures Working Group
March 2009 - January 2010	CBUFA-CBU Association-Employer Committee
July 2009 -	Vice Chair of Department of Chemistry
July 2009 – June 2010	Chair of School of Science and Technology
Sept. 2010 -	Research Assistance Committee
Jan. 2011 -	Chemistry Curriculum Committee

OTHER ACADEMIC EXPERIENCE

Service at Scientific Conferences

Session chair and judge of graduate student talks, 80th Canadian Society for Chemistry Conference and Exhibition, June, 1997, Windsor, Ont.

Chair of judging of undergraduate student talks, 6^{th} Atlantic Theoretical Chemistry Symposium, August 2006, Antigonish, NS.

Session chair, 8th Atlantic Theoretical Chemistry Symposium, August, 2007, St. John's, NL.

Judge of graduate student posters in Physical Chemistry Division, 91st Canadian Chemistry Conference and Exhibition, May 2008, Edmonton, AB.

Organizer, 9th Atlantic Theoretical Chemistry Symposium, August, 2008, Sydney, NS.

Session chair, 10th Atlantic Theoretical Chemistry Symposium, July 2009, Fredericton, NB.

Chair of Poster Session, Coordinator of Poster Judging, 7th Canadian Computational Chemistry Conference, July 2009, Halifax, NS.

Session chair and judge of student talks, 12th Atlantic Theoretical Chemistry Symposium, August, 2011, Charlottetown, PEI.

HONOURS THESES EXAMINED (Supervisor's name in parentheses)

Scott Jaspers-Fayer (Dale Keefe) 2010/11.

Cara Andrews (Dale Keefe) 2010/11.

Zuzana Istvankova (Dale Keefe), 2009/10.

Kristen MacDonald (Matthias Bierenstiel), 2008/09.

Janet Pickup (Dale Keefe), 2008/09.

Merrill Isenor (Dale Keefe), 2006/07.

School Outreach Service

Wrote, proctored and graded Grade 9 Physical Science exam for 1998 North Central Arkansas Regional Mathematics and Science Competition.

Judged Junior High Chemistry for 1998 North Central Arkansas Regional Science Fair.

Served at the Annual High School Science Saturday, SUNY Potsdam, November 13, 1999, November 16, 2001.

Coordinated Chemistry Magic Show, Science and Technology Open House, Cape Breton University, November 5, 2005.

Judged Junior category projects, Cape Breton Regional Science Fair, March 26, 2008.

Judged Senior category projects, Cape Breton Regional Science Fair, March 25, 2009.

Judged Chemistry category projects, Cape Breton Regional Science Fair, March 30, 2010.

Presented at Science Rendezvous, Mayflower Mall, May 7, 2011.

Departmental Seminar Presentations

"Assessment of Basis Set and Functional Dependencies in Density Functional Theory: Canadian-Swedish Collaborations", June 12, 1996, Department of Physics, Stockholm University, Stockholm, Sweden.

"Assessment of Basis Set and Functional Dependencies in Density Functional Theory: Canadian-Swedish Collaborations", June 14, 1996, Department of Quantum Chemistry, Uppsala University, Uppsala, Sweden.

"Computational Studies of Halocarbon Reactions", February 26, 1998, Department of Chemistry, Lyon College, Batesville, AR.

"Computational Studies of Halocarbon Reactions: Past, Present, and Future", December 2, 1998, Department of Chemistry, UNC Asheville.

"Computational Studies of Halocarbon Reactions", February 22, 2000, Department of Chemistry, SUNY Potsdam, Potsdam, NY.

"Computational Studies of Some Atmospherically Significant (or Not) Reactions", March 20, 2009, Saint Mary's University, Halifax, NS.

Peer Reviewing

Refereed manuscripts for the following journals:

Journal of the American Chemical Society (1)
Journal of Physical Chemistry (3)
Canadian Journal of Chemistry (7)
Molecular Physics (1)
Acta Chemica Scandinavica (1)
Journal of Molecular Spectroscopy- THEOCHEM (11)
Computational and Theoretical Chemistry (3)

Chapter review for:

Chemistry: A Molecular Approach, by Nivaldo J. Tro An Introduction to Physical Chemistry, by William M. Davis

STUDENT AND PROFESSIONAL ASSOCIATIONS

Saint Mary's University Vice-President, 1988-89 Chemistry Society Treasurer, 1990-91

Departmental Representative, Summer 1989, 1990-91

Dalhousie Chemistry Graduate Student Seminar Coordinator, 1991-92 Graduate Students Society Safety Committee Representative, 1992-94

Canadian Society for Chemistry Member since 1990

Chemical Institute of Canada Treasurer, 2008-2011

Maritimes Local

Computational Chemistry Institute Treasurer, 2008-2011

of ACENet