Michelle M. Francl
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Research Interests

Theoretical and computational chemistry; development of methods to assess molecular reactivity; structures of topologically intriguing molecules; science writing

Positions Held

Bryn Mawr College

Professor of Chemistry	2001-present
Co-Director, Emily Balch Seminar Program	2009-present
Chair, Department of Chemistry	2005-2008
Director, Katharine Houghton Hepburn Center	2005-2007
Associate Professor of Chemistry	1992-2001
Assistant Professor of Chemistry	1986-1992

Visiting Appointments

Lawrence Livermore National Laboratory (Physicist)	1998-1999
Princeton University (Visiting Fellow)	1992-1993
James Franck Institute, University of Chicago (Visiting Fellow)	1992
Haverford College (Assistant Professor of Chemistry)	1985-1986

Current Professional Activities

Columnist, *Nature Chemistry* (2009-present)
Board of Examiners, Chemistry GRE (2008-present)
Nominations & Elections Committee, American Chemical Society (2006-2008)
OXIDE (Open Chemistry Collaborative in Diversity Equity) Advisory Board (2010-)

Education

Postdoctoral Fellow, Princeton University	1983-1985
Ph.D. (Chemistry), University of California, Irvine	1983
B.S. (Chemistry),University of California, Irvine	1979

Awards and Distinctions

Fellow of the American Chemical Society	(elected 2009)
McPherson Fellowship, Bryn Mawr College	2003
ISI List of Top 1000 Most Cited Chemists	1981-97
Christian R. and Mary F. Lindback Award	1994
Rosalyn R. Schwartz Lectureship	1987-1991

Recent Professional Activities

Member of the American Chemical Society Council, representing COMP (1999-2007)
Past Chair, Computers in Chemistry Division of the American Chemical Society (2005)
Board Oversight Group on Leadership Development, American Chemical Society (2004-2009)
Editorial Board, *Journal of Molecular Graphics and Modelling* (1998-2006)
Chair, Computers in Chemistry Division of the American Chemical Society (2004)
Chair-Elect, Computers in Chemistry Division of the American Chemical Society (2003)
Divisional Activities Committee, Vice-Chair, American Chemical Society Council (2005)
Divisional Activities Committee, Secretary, American Chemical Society Council (2003-2004)
Divisional Activities Committee, American Chemical Society Council (2000-2005)

Recent College Service

Curriculum Committee, 2008-2009
Abu Dhabi Working Group, Chair, 2008
College Seminar Steering Committee, 1998-2007
Faculty Grand Marshal (2000-2006)

Current Funding

"Emerging Frontiers of Science of Information", NSF (multi-institutional grant)

Publications

Articles and Book Chapters

1. Self-Consistent Molecular Orbital Methods. 23. A Polarization Basis Set for Second Row Elements, M.M. Francl, W.J. Pietro, W.J. Hehre, J.S. Binkley, D.J. DeFrees, J.A. Pople and M.S. Gordon, *J. Chem. Phys.* **77**, 3654-3665 (1982).

2. Self-Consistent Molecular Orbital Methods. 24. Supplemented Small Split-Valence Basis Sets for Second Row Elements, W.J. Pietro, M.M. Francl, W.J. Hehre, J.S. Binkley, D.J. DeFrees, and J.A. Pople *J. Amer. Chem. Soc.* **104**, 5039-5048 (1982).

3. Conformational Preferences in Transition Metal Carbenes, M.M. Francl, W.J. Pietro, R.F. Hout, Jr. and W.J. Hehre, *Organometallics* **2**, 815-818 (1983).

4. Hyperconjugation and the Structures of Metal Carbenes, M.M. Francl, W.J. Pietro, R.F. Hout, Jr., and W.J. Hehre, *Organometallics* **2**, 281-286 (1983).

5. The Structure of the Tebbe Reagent. An Intramolecular Complex?, M.M. Francl and W.J. Hehre, *Organomet.* **2**, 457-459 (1983).

6. Conformational Preferences in Mo_2L_6 Complexes, K.D. Dobbs, M.M. Francl and W.J. Hehre, *Inorg. Chem.* **23**, 24-26 (1984).

7. Representation of Electron Densities. 1. Sphere Fits to Total Electron Density Surfaces, M.M. Francl, R.F. Hout, Jr., and W.J. Hehre, *J. Amer. Chem. Soc.* **106**, 563-570 (1984).

8. Role of Active-Site Residues and Solvation in RNase-A, C. Brooks III, A. Brunger, M.M. Francl, K. Haydock, L.C. Allen and M. Karplus, *Ann. N.Y. Acad. Sci.* **471**, 295-298 (1986).

9. Polarization Corrections to Electrostatic Potentials, M.M. Francl, *J. Phys. Chem.* **89**, 428-433 (1985).

10. Anionic Hyperconjugation, D.S. Friedman, M.M. Francl and L.C. Allen, *Tetrahedron* **41**, 499-506 (1985).

11. Charges Fit to Electrostatic Potentials, L.E. Chirlian and M.M. Francl, *J. Comp. Chem.* **8**, 894-905 (1987).

12. The Stability of Rotational Transition Structures in Substituted Amides, K.T. Lim and M.M. Francl, *J. Phys. Chem.* **91**, 2716-2721 (1987).

13. Phosphoranes: Bond Characterization and Substituent Effects, M.M. Francl, R.C. Pellow and L.C. Allen, *J. Amer. Chem. Soc.* **110**, 3723-3728 (1988).

14. Isomers of Nitric Acid and Chlorine Nitrate, M.P. McGrath, M.M. Francl, F.S. Rowland and W.J. Hehre, *J. Phys. Chem.* **92**, 5352-5357 (1988).

15. π- complexes of Alkenes to Trivalent Aluminum, J. Chey, H.S. Choe, Y.M. Chook, E. Jensen, P.R. Seida and M.M. Francl, *Organometallics* **9**, 2430-36 (1990).

16. The N_4 Molecule and its Metastability, M.M. Francl and J.P. Chesick, *J. Phys. Chem.* **94**, 526-528 (1990).

17. 1-Oxabicyclobutonium Ions Can Intervene in Epoxycarbinyl and 3-Oxetanyl Solvolysis, M.M. Francl, G. Hansell, B.P. Patel and C.S. Swindell, *J. Amer. Chem. Soc.* **112**, 3535-3539 (1990).

18. A Theoretical Investigation of Aluminum-Oxygen π-Bonding in 3- and 4-Coordinate Aluminum Alkoxides, A. R. Barron, K. D. Dobbs and M. M. Francl, *J. Amer. Chem. Soc.* **113**, 39-43 (1991).

19. Computational Studies of Structure and Bonding in Organoaluminum Complexes, A. Shaw, P.R. Seida, J.W. Bundens and M.M. Francl in Topics in Physical Organometallic Chemistry, vol. 4, pg. 353-393 (1992).

20. Transition States for Hydroalumination of Alkenes and Alkynes: Ab Initio Molecular Orbital Studies, J.W. Bundens and M. M. Francl *Organometallics* **12**, 1608-1615 (1993).

21. NMR and Molecular Modeling Study of the Conformations of Taxol and of its Side Chain Methylester in Aqueous and Non-Aqueous Solution, H.J. Williams, A.I. Scott, R.A. Dieden, C.S. Swindell, L.E. Chirlian, M.M. Francl, J.M. Heerding, N.E. Krauss, *Tetrahedron* **49**, 6545-6569 (1993).

22. Distance Dependence of Nonadiabaticity in the Branching Between C-Br and C-Cl Bond Fission following $^1n(O)\rightarrow\pi^*(C=O)$ Excitation in Bromopropionyl Chloride, P.W. Kash, G. C. G. Waschewsky, L. J. Butler, M. M. Francl, *J. Chem. Phys.* **99**, 4479-4494 (1993).

23. NMR And Molecular Modeling Study Of Active And Inactive Taxol Analogs In Aqueous And Nonaqueous Solution, H.J. Williams, A.I. Scott, R.A. Dieden, C.S. Swindell, L.E. Chirlian, M.M. Francl, J.M. Heerding, N.E. Krauss, *Can. J. Chem.* **72**, 252-260 (1994).

24. Competing C-Br and C-C Bond Fission following $^1[n(O),\pi^*(C=O)]$ Excitation in Bromoacetone: Conformation Dependence of Nonadiabaticity at a Conical Intersection, P.W. Kash, G. C. G. Waschewsky, R.E. Morrs, L. J. Butler, M. M. Francl, *J. Chem. Phys.* **100**, 3463-3475 (1994).

25. Charges Fit to Electrostatic Potentials II: Can Atomic Charges be Unambiguously Fit to Electrostatic Potentials?, C. Carey, L.E. Chirlian, D. Gange and M.M. Francl, *J. Comp. Chem.* **17**, 367-383 (1996).

26. Beyond CHELP: Improved Potential Derived Charges for Sugars, C. Carey, L.E. Chirlian, D. Gange and M.M. Francl, *Glycoconjugate Journal* **14**, 501-505 (1997).

27. Transition States for the Carboalumination of Alkene and Alkynes, J.W. Bundens, J. Yudenfreund and M.M. Francl, *Organometallics* **18**, 3913-3920 (1999).

28. The Pluses and Minuses of Mapping Atomic Charges to Electrostatic Potentials, M.M. Francl and L.E. Chirlian, in *Rev. in Computational Chem.* **14**, 1-31 (2000).

29. Nuclear Spin-Spin Coupling via Nonbonded Interactions. 8.1 The Distance Dependence of Through-Space Fluorine-Fluorine Coupling, F.B. Mallory, C.W. Mallory, K.E. Butler, M.B. Lewis, A.Q. Xia, E.D. Luzik, Jr., L.E. Fredenburgh, M.M. Ramanjulu, Q.N. Van, M.M. Francl, D.A. Freed, C.C. Wray, C. Hann, M. Nerz-Stormes, P.J. Carroll, and L.E. Chirlian, *J. Amer. Chem. Soc.* **122**, 4108-4116 (2000).

30. An Ab Initio MO Study of the Symmetric And Asymmetric Isomers of Bridging Alkynylaluminum and Alkynylberyllium Dimers, P. R. Seida, J.W. Bundens, M.M. Francl, *International Journal of Quantum Chemistry*, **95**, 806-809 (2003).

31. Exploring Exotic Kinetics: An Introduction to the Use of Numerical Methods in Chemical Kinetics, M. M. Francl *Journal of Chemical Education*, **81**, 1535 (2004).

32. Introduction to Statistical Mechanics, M.M. Francl, *Journal of Chemical Education*, **82**, 175 (2005).

33. Elemental MoThEr. M. M. Francl, in *Parenting and Professing: Balancing Family Work with an Academic Career*, ed. Rachel Hile-Basset, Vanderbilt University Press, June 2005.

34. Crossing the Line: Stochastic Methods in the Chemistry Curriculum, M.M. Francl in *Annual Reports in Computational Chemistry* v. 1, ed. D. Spellmeyer, Elsevier, 2005.

35. A Theoretical Study of the Reduction Of Carbonyls By Alkylaluminum Complexes, J.W. Bundens, P.R. Seida, D. Jeyakumar and M.M. Francl, *Journal of Molecular Graphics and Modeling*, **24**, 195-202 (2005).

36. CF_3 Rotation in 3-trimethylfluorophenanthrene: X-ray Diffraction and ab initio Electronic Structure Calculations, X. Wang, F.B. Mallory, C.W. Mallory, A.J. Rheingold, P.A. Beckmann, M.M. Francl, *J. Phys. Chem. A*, **110**, 3954-3960 (2006).

37. Walking the Tightrope: Teaching the timeless fundamentals in the context of modern physical chemistry, M.M. Francl In *Advances in Teaching Physical Chemistry*; Ellison, M., Schoolcraft, T., Eds.; ACS Symposium Series 973; American Chemical Society: Washington, DC, 2007; pp 253-267.

38. Table manners, M.M. Francl, *Nature Chemistry*, **1**, 97-98 (2009).

39. Stretching topology, M.M. Francl, *Nature Chemistry*, **1**, 97-98 (2009).

40. Mapping the two cultures, M.M. Francl, *Nature Chemistry*, **1**, 591-592 (2009).

41. Back to basics, M.M. Francl, *Nature Chemistry*, **1**, 681 (2009).

42. Men of mystery, M.M. Francl, *Nature Chemistry*, **2**, 68-70 (2010).

43. Pressure to Preserve, M.M. Francl in *Open Laboratory 2009*, B. Zivkovic and Scicurious, eds., 2010.

44. Staging science, M.M. Francl, *Nature Chemistry*, **2**, 238-239 (2010).

45. Urban legends of chemistry, M.M. Francl, *Nature Chemistry*, **2**, 600-601 (2010).

46. Science for sale, M.M. Francl, *Nature Chemistry*, in press (December 2010).

Books

Thinking Like a Scientist: A Field Guide to the Natural World, O'Reilly Press, under contract.
ACS Physical Chemistry Examination Study Guide, ACS Examinations Institute, 2010
A Survival Guide for Physical Chemistry, M.M. Francl, Physics Curriculum & Instruction Press, 2001.

Other writing

Literature Reviews for *Chemical Design and Automation News*:
June 1993, September 1993, April 1994, June 1994 , Fall 1994, January/February 1995, August 1995, January/February 1996, Fall 1996

Culture of Chemistry
Short essays on aspects of chemistry hosted at http://cultureofchemistry.blogspot.com
Approximate circulation: 3200 unique readers per month.

Columnist, *Catholic Standard & Times* (2008-present)

Computer Programs

1. GAUSSIAN 85, R.F. Hout, Jr., M.M. Francl, N. Blurock, W.J. Pietro, S.K. Pollack, D.J. DeFrees, B.A. Levi, R. Steckler, W.J. Hehre.
2. MEPHISTO, M.M. Francl, Quantum Chemistry Program Exchange, Program 490, 1984.
3. CHELP, L.E. Chirlian and M.M. Francl, Quantum Chemistry Program Exchange, Program 594, 1988.
4. Quantum Chemistry Graphics Archive, P.R. Seida and M.M. Francl, 1990.
5. MOPC, P.R. Seida and M.M. Francl, Quantum Chemistry Program Exchange, Program QCMP090, 1991.
6. CHELP-SVD , L.E. Chirlian and M.M. Francl, 1996.

Curricular Materials

Multimedia

Introduction to Quantum Mechanics, a full semesters worth of lectures, available from *iTunes* as audio and at http://chemistry221.blogspot.com as video

Mathematica

1. "Introduction to the Use of Numerical Methods in Chemical Kinetics", M.M. Francl, *MathSource*, Wolfram, Inc, 2000. www.mathsource.com

2. "Introduction to Statistical Mechanics", M.M. Francl, *MathSource*, Wolfram, Inc, 2000. www.mathsource.com

3. "Exploring Exotic Kinetics: An Introduction to the Use of Numerical Methods in Chemical Kinetics" M. M. Francl, c. 2004, available from *JCE SymMath* at http://jchemed.chem.wisc.edu/JCEDLib/SymMath/collection/index.html (Please note this material is peer reviewed.)

4. "An Introduction to Statistical Mechanics" M. M. Francl, c. 2005 available from *JCE SymMath* at http://jchemed.chem.wisc.edu/JCEDLib/SymMath/collection/index.html (Please note this material is peer reviewed.)

P-Chem with a Purpose (funded by NSF-DUE)

Overview at http://www.brynmawr.edu/Acads/Chem/NSFpchem/
Modules at http://www.brynmawr.edu/Acads/Chem/NSFpchem/DraftModules.html

1. Miniature Machines: "Pulling" Nanowires

2. Frog Antibiotics: Statistical Mechanics of Helix-Coil Transitions

3. Ancient Ostrich Eggs: Dating Materials By Amino Acid Racemization

4. Quantum Dots: Particle-on-a-sphere model for Buckminsterfullerene

5. Using Chemistry to Uncover a History: Is this an early map of North America – or not?

6. Exotic Kinetics: Oscillating Reactions in the Atmosphere

Recent Invited Lectures

"Practical Approaches to the Impractical/Impractical Approaches to the Practical," October 2009, Association for the Contemplative Mind in Higher Education (archived at http://vimeo.com/7223309)

"Contemplative practices in the science classroom, " 5th Annual Summer Session on Contemplative Curriculum, August 2009

"The fruits of monasticism in the classroom, " Fetzer Institute, October 2008

"Physical chemistry materials for the 21st century: Squids to stat mech" American Chemical Society National Meeting, March 2006

"Walking the tightrope: Finding the timeless fundamentals in the context of modern physical chemistry" American Chemical Society National Meeting, August 2005

"Replacing the Blackboard: Using *Mathematica* to Teach Modern Chemical Kinetics" American Chemical Society National Meeting, August 2005

"Move Away from the Chalkboard: Restructuring the Physical Chemistry Lecture" Drexel University, May 2005.

"A Quantum Chemist Looks Under the Hood: What Makes Molecules Do the Things They Do?" Princeton Plasma Physics Lab,, January 2005.