

Curriculum Vitae

Sharon Hammes-Schiffer

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Date of Birth May 27, 1966

Education

B.A.	Chemistry	Princeton University	5/88
	summa cum laude, Highest Honors in Chemistry		
Ph.D.	Chemistry	Stanford University	9/93
	Graduate advisor: Hans C. Andersen		

Professional Experience

Eberly Professor in Biotechnology Pennsylvania State University	8/06 - present
Professor of Chemistry Pennsylvania State University	7/03 - present
Shaffer Associate Professor of Chemistry Pennsylvania State University	8/00 - 7/03
Clare Boothe Luce Assistant Professor of Chemistry University of Notre Dame	8/95 - 8/00
Postdoctoral research scientist AT&T Bell Laboratories AT&T Bell Laboratories, Murray Hill, NJ Postdoctoral supervisor: John C. Tully	9/93 - 8/95

Honors and Awards

William Foster Memorial Prize in Chemistry, Princeton University, 1987
American Institute of Chemists Student Award, 1988
Merck Index Award, Princeton University, 1988
ACS Regional Scholarship Award, 1988
AT&T Bell Laboratories GRPW (Graduate Research Program for Women) Grant, 1988-92
NSF Graduate Fellowship in Chemistry, 1988-91
NSF CAREER Award, 1996
Ralph E. Powe Junior Faculty Enhancement Award, Oak Ridge Associated Universities, 1998
Alfred P. Sloan Research Fellowship, 1998
Camille Dreyfus Teacher-Scholar Award, 1999
NSF Creativity Extension Award, 2003
Alexander M. Cruickshank Lecturer, Gordon Research Conference on Isotopes in Biological & Chemical Sciences, 2004
Ephraim and Wilma Shaw Roseman Lecturer, Johns Hopkins University, 2004
Lucy Pickett Lecturer, Mount Holyoke College, 2004
Donald Lecturer, McGill University, 2004

Honors and Awards (continued)

Woodward Lecturer, Harvard University, 2004
Iota Sigma Pi Agnes Fay Morgan Research Award, 2005
International Academy of Quantum Molecular Science Medal, 2005
American Chemical Society Akron Section Award, 2008

Professional Service

Senior Editor for *The Journal of Physical Chemistry*, 2001 – present
Rotation as Chair of the Physical Chemistry Division of the American Chemical Society, 2008 – 2013
Editorial Advisory Board for *The Journal of the American Chemical Society*, 2008 – 2010
Editorial Advisory Board for *Accounts of Chemical Research*, 2006 – present
Member of BESAC (Basic Energy Sciences Advisory Committee) for the Department of Energy, 2008 – 2010
Guest Editor for a special issue of *Accounts of Chemical Research* on Artificial Photosynthesis and Solar Fuels, 2009
Guest Editor for a special issue of *Chemical Reviews* on Proton-Coupled Electron Transfer, 2010
Advisory Board for *Theoretical Chemistry Accounts*, 2002 – 2008
Member of a Committee of Visitors (COV) for the Chemical Sciences, Geosciences, and Biosciences Division in Basic Energy Sciences, serving on a panel that covers the research activities in the Photochemistry and Radiation Research and Condensed-phase Chemical Physics programs, April 2008
Co-organizing a Workshop on Chemical Dynamics: Challenges and Approaches for a Thematic Year in Mathematics and Chemistry at the Institute for Mathematics and its Applications at the University of Minnesota, January 2009
Organized the symposium entitled “Quantum Mechanics and Statistical Mechanics: Can One Avoid the Other?” for the American Chemical Society National Meeting in August, 2007 in Boston, MA
Organized the symposium entitled “Computational Studies of Mechanistic and Dynamical Aspects of Enzyme Reactions” for the ASBMB meeting in May, 2007 in Washington D.C.
Charter Member of the MSFA NIH study section, 2004 – 2006
Charter Member of the BBFA NIH study section, 2002 – 2004
Vice-Chair/Chair, Theoretical Subdivision of the American Chemical Society, 2002 – 2005
Co-organized the symposium on Quantum/Classical Calculations in Chemistry and Biophysics for the American Chemical Society National Meeting in August, 2004
Co-organized the CECAM workshop on Methods for Computer Simulation of Nonadiabatic Charge Transfer Processes in the Condensed Phase in Lyon, France in April, 2002
Served on NIH review panels: March 11, 1999; February 11, 2000; August 1, 2001
Organized the symposium on Proton Transport in Liquids, Solids, and Proteins for the American Chemical Society National Meeting in August, 2000
Co-organized the Midwest Theoretical Chemistry Conference at the University of Notre Dame in May, 1999
Organized the Telluride Workshop on Condensed Phase Dynamics in Telluride, Colorado in July, 1998
Served on the panel for NSF CAREER Awards in physical chemistry in November, 1998
Refereed papers for *Journal of Chemical Physics*, *Journal of Physical Chemistry*, *Chemical Physics Letters*, *Biophysical Journal*, *Journal of the American Chemical Society*, *Journal of Computational Chemistry*, *Chemical Physics*, and others

Refereed proposals for the National Science Foundation, the ACS Petroleum Research Fund, the Department of Energy and others

Membership in Professional Organizations

Phi Beta Kappa, Sigma Xi, American Association for the Advancement of Science,
American Chemical Society

Students and Postdocs Supervised

Current Graduate Students

Dhruva Chakravorty, Laura Fernandez, Philip Hanoian, Sarah Hillard, Michelle Ludlow, Ran Tu, Narayanan Veeraraghavan

Current Postdoctoral Research Assistants

Ben Auer, Anirban Hazra, Charulatha Venkataraman
Michael Pak (Research Associate), Chet Swalina (Research Associate), Alexander Soudackov (Research Assistant Professor)

Current Undergraduate Student

Tyler Garner

Past Graduate Students

John Morelli, M.S., University of Notre Dame, 1999

current position: President and CEO of Nuron, sold to Intel in 2001; Founder and Chairman of Coaxsys

Hong Hu, M.S., University of Notre Dame, 2000

Karen Drukker, Ph.D., University of Amsterdam (University of Notre Dame), 1998

current position: Research Associate and Assistant Professor, Department of Radiology,
University of Chicago

Hélène Decornez, Ph.D., Pennsylvania State University, 2001

current position: Senior Research Chemist, Computer-Aided Drug Discovery,
Albany Molecular Research, Inc.

Pratul Agarwal, Ph.D., Pennsylvania State University, 2002

current position: Staff Scientist at Oak Ridge National Laboratory; Adjunct Faculty in Graduate Program
in Genome Science and Technology at University of Tennessee

Nedialka Iordanova, Ph.D., Pennsylvania State University, 2003

current position: Associate Professor, Department of Chemistry, Georgia Southwestern University

Tzvetelin Iordanov, Ph.D., Pennsylvania State University, 2003

current position: Associate Professor, Department of Chemistry, Georgia Southwestern University

James Watney, Ph.D., Pennsylvania State University, 2005

current position: Technical Support Scientist at Schrodinger, Inc.

Soo Young Kim, Ph.D., Pennsylvania State University, 2006

Chet Swalina, Ph.D., Pennsylvania State University, 2006

current position: Research Associate faculty position at Pennsylvania State University

Elizabeth Hatcher, Ph.D., Pennsylvania State University, 2006

current position: postdoc at University of Maryland, Baltimore

Yolanda Small, Ph.D., Pennsylvania State University, 2007

current position: postdoc at Brookhaven National Lab

Jonathan Skone, Ph.D., Pennsylvania State University, 2008

current position: postdoc at Brookhaven National Lab

Malika Kumarasiri, Ph.D., Pennsylvania State University, 2008

current position: postdoc at University of Notre Dame

Past Postdoctoral Research Assistants

Margaret Hurley, January 1996-June 1997

current position: Computational and Information Sciences Directorate, US Army Research Laboratory

Jian-Yun Fang, June 1996-June 1999

Atul Bahel, January 1999-May 2000

Alexander Soudackov, April 1998-June 2000

current position: research assistant professor at Penn State

Ivan Rostov, July 1999-June 2001

current position: computational chemist, supercomputer facility, Australian National University

Salomon Billeter, November 1999-June 2001

current position: research scientist at IBM Zurich

Mark Kobrak, January 2000-August 2001

current position: associate professor at CUNY Brooklyn

Simon Webb, August 1998-December 2001

current position: research scientist at VeraChem

Claudio Carra, August 2001- June 2003

current position: research scientist at NASA

Kim Fay Wong, October 2001 - July 2004

current position: postdoctoral researcher at University of Utah

Alessandro Sergi, August 2004 – March 2005

current position: assistant professor at University of KwaZulu-Natal

Andres Reyes, July 2003 – June 2005

current position: assistant professor in Columbia

Qian Wang, August 2005 – August 2006

current position: postdoctoral researcher at Purdue University

Yasuhito Ohta, November 2004 – November 2006

current position: research associate at Kyoto University

Hiroshi Ishikita, November 2005 – November 2007

current position: assistant professor at University of Tokyo

Irina Navrotskaya, January 2007 - February 2009

current position: postdoc with Will Noid at Pennsylvania State University

Arindam Chakraborty, March 1, 2006 - August 2009

current position: assistant professor at Syracuse University

Past Undergraduate Research Assistants

Susan McGovern, Michael Niemier, Charles Vardeman (University of Notre Dame), Jeff Meadows, Greg Baker

Research Funding

Completed

National Science Foundation CAREER Award The Incorporation of Quantum Effects in the Simulation of Proton Transfer Reaction	6/1/96 - 5/31/00	\$235,700
Petroleum Research Fund (administered by ACS) Simulation of Proton Transport along a Linear Chain of Hydrogen-Bonded Water Molecules	9/1/96 - 8/31/98	\$20,000
Air Force Office of Scientific Research Simulation of Reaction Dynamics: Nonadiabatic and Solvation Effects	2/1/98 - 11/30/00	\$322,042
Oak Ridge Associated Universities Ralph E. Powe Junior Faculty Enhancement Award	6/1/98 - 5/31/99	\$10,000
Alfred P. Sloan Foundation Research Fellowship	9/16/98 - 9/15/02	\$35,000
National Institutes of Health Simulation of Proton and Hydride Transfer in Enzymes	5/1/98 - 4/30/03	\$779,607
Camille Dreyfus Teacher-Scholar Award	6/1/99 - 5/31/04	\$60,000
Air Force Office of Scientific Research Simulation of Reaction Dynamics for Synthesis of Energetic Materials and Resistant Coatings	12/1/00 - 11/30/03	\$345,000
National Science Foundation Theoretical and Computational Studies of Multiple Charge Transfer Reactions in the Condensed Phase	6/1/00 - 5/31/04	\$385,000
National Science Foundation Creativity Extension	6/1/04 - 5/31/05	\$140,000
Air Force Office of Scientific Research Simulation of Reactions for the Design of Energetic Materials, Resistant Coatings, and Laser Protection Devices	1/1/04 - 12/31/06	\$381,926
National Institutes of Health Simulation of Proton and Hydride Transfer in Enzymes: Supplement	1/1/04 - 12/31/06	\$139,504
National Institutes of Health Simulation of Proton and Hydride Transfer in Enzymes	5/1/03 - 4/30/07	\$921,832
DOD PET Program Porting the Nuclear-Electronic Orbital (NEO) Method to the GAMESS Code for Air Force Applications	8/1/06 - 7/31/07	\$60,000
DARPA Evolution-Based Design of Allosteric Control Systems in Proteins (group proposal, P.I. Rama Ranganathan)	1/1/07 - 12/31/07	\$91,710 (S.H.S.)
DARPA New Technology for Inside-Out Design of Novel Enzyme Catalysts (group proposal, P.I. David Baker)	7/11/05 - 12/14/07	\$234,980 (S.H.S.)
National Science Foundation Theoretical Studies of Proton-Coupled Electron Transfer Reactions	7/1/05 - 6/30/08	\$415,000
Department of Energy	10/1/05 - 9/30/08	\$114,725 (S.H.S.)

Nanoscale Building Blocks for Multi-Electron Electrocatalysis: The Oxygen Reduction Reaction in Fuel Cells and Oxygen Evolution in Water Electrolysis (in collaboration with ORNL, P.I. Gilbert Brown)

Current

National Science Foundation Theoretical Studies of Proton-Coupled Electron Transfer Reactions	7/1/08 - 6/30/11	\$440,000
Air Force Office of Scientific Research Development of the Nuclear-Electronic Orbital Approach and Applications to Ionic Liquids and Tunneling Processes	1/1/07 - 11/30/09	\$504,000
Air Force Office of Scientific Research Development of the Nuclear-Electronic Orbital Approach and Applications to Water-Anion Complexes and Biomimetic Models of Hydrogenase	12/1/09 - 11/30/13	\$750,207
National Institutes of Health Simulation of Proton and Hydride Transfer in Enzymes	5/1/07 - 4/30/11	\$1,022,039
National Institutes of Health Simulation of Proton and Hydride Transfer in Enzymes, Administrative Supplement	6/1/09 – 4/30/11	\$183,309
National Science Foundation An Integrative Approach to Metalloenzyme-Catalyzed C-H Activation (group proposal with J. M. Bollinger and C. Krebs, NSF-DFG program)	8/15/07 - 7/31/10	\$183,000 (S.H.S.)
National Science Foundation Powering the Planet: A Chemical Bonding Center in the Direct Conversion of Sunlight into Chemical Fuel (group proposal, P.I. Harry Gray)	8/1/08 - 7/31/13	\$881,078 (S.H.S.)
Department of Energy Center for Molecular Electrocatalysis (group proposal, P.I. Morris Bullock)	8/1/09 – 7/30/14	\$1,125,000 (S.H.S.)

Publications

1. F. Loaiza, M. A. McCoy, S. L. Hammes, and W. S. Warren, "Selective excitation without phase distortion using self-refocused amplitude- and amplitude/phase-modulated pulses," *J. Mag. Res.* **77**, 175-181 (1988).
2. A. Hasenfeld, S. L. Hammes, and W. S. Warren, "Understanding of phase modulation in two-level systems through inverse scattering," *Phys. Rev. A* **38**, 2678-2681 (1988).
3. W. S. Warren, S.L. Hammes, and J. L. Bates, "Dynamics of radiation damping in nuclear magnetic resonance," *J. Chem. Phys.* **91**, 5895-5904 (1989).
4. S. L. Hammes, L. Mazzola, S. G. Boxer, D. F. Gaul, and C. C. Schenck, "Stark spectroscopy of the Rhodobacter sphaeroides reaction center heterodimer mutant," *Proc. Natl. Acad. Sci.* **87**, 5682-5686 (1990).
5. S. Han, Y-C. Ching, S. L. Hammes, and D. L. Rousseau, "Vibrational structure of the formyl group on heme A: Implications on the properties of cytochrome c oxidase," *Biophys. J.* **60**, 45-52 (1991).
6. D. J. Lockhart, S. L. Hammes, S. Franzen, and S. G. Boxer, "Electric field effects on emission line shapes when electron transfer competes with emission: An example from photosynthetic reaction centers," *J. Phys. Chem.* **95**, 2217-2226 (1991).
7. S. Hammes-Schiffer and H. C. Andersen, "Ab initio and semiempirical methods for molecular dynamics simulations based on general Hartree-Fock theory," *J. Chem. Phys.* **99**, 523-532 (1993).
8. S. Hammes-Schiffer and H. C. Andersen, "The advantages of the general Hartree-Fock method for future computer simulation of materials," *J. Chem. Phys.* **99**, 1901-1913 (1993).
9. S. Hammes-Schiffer and H. C. Andersen, "A new formulation of the Hartree-Fock-Roothaan method for electronic structure calculations on crystals," *J. Chem. Phys.* **101**, 375-393 (1994).
10. S. Hammes-Schiffer and J. C. Tully, "Proton transfer in solution: Molecular dynamics with quantum transitions," *J. Chem. Phys.* **101**, 4657-4667 (1994).
11. S. Hammes-Schiffer and J. C. Tully, "Vibrationally enhanced proton transfer," *J. Phys. Chem.* **99**, 5793-5797 (1995).
12. S. Hammes-Schiffer and J. C. Tully, "Nonadiabatic transition state theory and multiple potential energy surface molecular dynamics of infrequent events," *J. Chem. Phys.* **103**, 8528-8537 (1995).
13. S. Hammes-Schiffer, "Multiconfigurational molecular dynamics with quantum transitions: Multiple proton transfer reactions," *J. Chem. Phys.* **105**, 2236-2246 (1996).
14. J. Morelli and S. Hammes-Schiffer, "Surface hopping and fully quantum dynamical wavepacket propagation on multiple coupled adiabatic potential surfaces for proton transfer reactions," *Chem. Phys. Lett.* **269**, 161-170 (1997).
15. J.-Y. Fang and S. Hammes-Schiffer, "Proton-coupled electron transfer reactions in solution: molecular dynamics with quantum transitions for model systems," *J. Chem. Phys.* **106**, 8442-8454 (1997).
16. M. M. Hurley and S. Hammes-Schiffer, "Development of a potential surface for simulation of proton and hydride transfer in solution: Application to NADH hydride transfer," *J. Phys. Chem. A* **101**, 3977-3989 (1997).
17. K. Drukker and S. Hammes-Schiffer, "An analytical derivation of MC-SCF vibrational wavefunctions for the quantum dynamical simulation of multiple proton transfer reactions: Initial application to protonated water chains," *J. Chem. Phys.* **107**, 363-374 (1997).
18. J.-Y. Fang and S. Hammes-Schiffer, "Excited state dynamics with nonadiabatic transitions for model photoinduced proton-coupled electron transfer reactions," *J. Chem. Phys.* **107**, 5727-5739 (1997).
19. J.-Y. Fang and S. Hammes-Schiffer, "Nonadiabatic dynamics for processes involving multiple avoided curve crossings: Double proton transfer and proton-coupled electron transfer reactions," *J. Chem. Phys.* **107**, 8933-8939 (1997).

20. H. Decornez, K. Drukker, M. M. Hurley, and S. Hammes-Schiffer, "Proton transport along water chains and NADH hydride transfer in solution," *Ber. Bunsenges. Phys. Chem.* **102**, 533-543 (1998) (special issue on hydrogen transfer).
21. K. Drukker, S. de Leeuw, and S. Hammes-Schiffer, "Proton transport along water chains in an electric field," *J. Chem. Phys.* **108**, 6799-6808 (1998).
22. J.-Y. Fang and S. Hammes-Schiffer, "Time-dependent self-consistent-field dynamics based on a reaction path Hamiltonian I. Theory," *J. Chem. Phys.* **108**, 7085-7099 (1998).
23. J.-Y. Fang and S. Hammes-Schiffer, "Time-dependent self-consistent-field dynamics based on a reaction path Hamiltonian II. Numerical tests," *J. Chem. Phys.* **109**, 7051-7063 (1998).
24. S. Hammes-Schiffer, "Mixed quantum/classical dynamics of single proton, multiple proton, and proton-coupled electron transfer reactions in the condensed phase," pp. 73-119 in *Comparisons of Classical and Quantum Dynamics, Volume III of Advances in Classical Trajectory Methods*, ed. W. L. Hase (JAI Press, Inc., Greenwich, 1998).
25. S. Hammes-Schiffer, "Quantum dynamics of multiple modes for reactions in complex systems," *Faraday Discuss. Chem. Soc.* **110**, 391-406 (1998).
26. S. Hammes-Schiffer, "Mixed quantum/classical dynamics of hydrogen transfer reactions" (Feature Article), *J. Phys. Chem. A* **102**, 10443-10454 (1998).
27. A. V. Soudackov and S. Hammes-Schiffer, "Removal of the double adiabatic approximation for proton-coupled electron transfer reactions in solution," *Chem. Phys. Lett.* **299**, 503-510 (1999).
28. H. Decornez, K. Drukker, and S. Hammes-Schiffer, "Solvation and hydrogen-bonding effects on proton wires," *J. Phys. Chem. A* **103**, 2891-2898 (1999).
29. J.-Y. Fang and S. Hammes-Schiffer, "Comparison of surface hopping and mean field approaches for model proton transfer reactions," *J. Chem. Phys.* **110**, 11166-11175 (1999).
30. A. Soudackov and S. Hammes-Schiffer, "Multistate continuum theory for multiple charge transfer reactions in solution," *J. Chem. Phys.* **111**, 4672-4687 (1999).
31. H. Decornez and S. Hammes-Schiffer, "Effects of model protein environments on the dynamics of proton wires," *Israel J. Chem.* **39**, 397-407 (1999) (special issue on Proton Solvation and Proton Mobility).
32. J.-Y. Fang and S. Hammes-Schiffer, "Improvement of the internal consistency in trajectory surface hopping," *J. Phys. Chem. A* **103**, 9399-9407 (1999).
33. A. Soudackov and S. Hammes-Schiffer, "Theoretical study of photoinduced proton-coupled electron transfer through asymmetric salt bridges," *J. Am. Chem. Soc.* **121**, 10598-10607 (1999).
34. P. K. Agarwal, S. P. Webb, and S. Hammes-Schiffer, "Computational studies of the mechanism for proton and hydride transfer in liver alcohol dehydrogenase," *J. Am. Chem. Soc.* **122**, 4803-4812 (2000).
35. H. Hu, M. N. Kobra, C. Xu, and S. Hammes-Schiffer, "Reaction path Hamiltonian analysis of dynamical solvent effects for a Claisen rearrangement and a Diels Alder reaction," *J. Phys. Chem. A* **104**, 8058-8066 (2000).
36. A. Soudackov and S. Hammes-Schiffer, "Derivation of rate expressions for nonadiabatic proton-coupled electron transfer reactions in solution," *J. Chem. Phys.* **113**, 2385-2396 (2000).
37. S. P. Webb, P. K. Agarwal, and S. Hammes-Schiffer, "Combining electronic structure methods with the calculation of hydrogen vibrational wavefunctions: Application to hydride transfer in liver alcohol dehydrogenase," *J. Phys. Chem. B* **104**, 8884-8894 (2000).
38. S. P. Webb and S. Hammes-Schiffer, "Fourier grid Hamiltonian multiconfigurational self-consistent-field: A method to calculate multidimensional hydrogen vibrational wavefunctions," *J. Chem. Phys.* **113**, 5214-5227 (2000).

39. H. Decornez and S. Hammes-Schiffer, "Model proton-coupled electron transfer reactions in solution: Predictions of rates, mechanisms, and kinetic isotope effects," *J. Phys. Chem. A* **104**, 9370-9384 (2000), featured on the cover.
40. S. Hammes-Schiffer, "Proton-coupled electron transfer," pp. 189-214 in *Electron Transfer in Chemistry Vol. I. Principles, Theories, Methods, and Techniques*, ed. V. Balzani (Wiley-VCH, Weinheim, 2001).
41. S. R. Billeter, S. P. Webb, T. Iordanov, P. K. Agarwal, and S. Hammes-Schiffer, "Hybrid approach for including electronic and nuclear quantum effects in molecular dynamics simulations of hydrogen transfer reactions in enzymes," *J. Chem. Phys.* **114**, 6925-6936 (2001).
42. T. Iordanov, S. R. Billeter, S. P. Webb, and S. Hammes-Schiffer, "Partial multidimensional grid generation method for efficient calculation of nuclear wavefunctions," *Chem. Phys. Lett.* **338**, 389-397 (2001).
43. S. Hammes-Schiffer, "Theoretical perspectives on proton-coupled electron transfer reactions," *Acc. Chem. Res.* **34**, 273-281 (2001).
44. N. Iordanova, H. Decornez, and S. Hammes-Schiffer, "Theoretical study of electron, proton, and proton-coupled electron transfer reactions in iron bi-imidazoline complexes," *J. Am. Chem. Soc.* **123**, 3723-3733 (2001).
45. I. Rostov and S. Hammes-Schiffer, "Theoretical formulation for electron transfer coupled to multiple protons: Application to amidinium-carboxylate interfaces," *J. Chem. Phys.* **115**, 285-296 (2001).
46. S. Hammes-Schiffer and S. Billeter, "Hybrid approach for the dynamical simulation of proton and hydride transfer in solution and proteins," *Int. Rev. Phys. Chem.* **20**, 591-616 (2001).
47. M. Kobraj and S. Hammes-Schiffer, "Molecular dynamics simulation of proton-coupled electron transfer in solution," *J. Phys. Chem. B* **105**, 10435-10445 (2001).
48. S. R. Billeter, S. P. Webb, P. K. Agarwal, T. Iordanov, and S. Hammes-Schiffer, "Hydride transfer in liver alcohol dehydrogenase: Quantum dynamics, kinetic isotope effects, and the role of enzyme motion," *J. Am. Chem. Soc.* **123**, 11262-11272 (2001).
49. S. Hammes-Schiffer, "Comparison of hydride, hydrogen atom, and proton-coupled electron transfer reactions," *ChemPhysChem* **3**, 33-42 (2002).
50. P. K. Agarwal, S. R. Billeter, P. T. R. Rajagopalan, S. J. Benkovic, and S. Hammes-Schiffer, "Network of coupled promoting motions in enzyme catalysis," *Proc. Nat. Acad. Sci. USA* **99**, 2794-2799 (2002).
51. P. K. Agarwal, S. R. Billeter, and S. Hammes-Schiffer, "Nuclear quantum effects and enzyme dynamics in dihydrofolate reductase catalysis," *J. Phys. Chem. B* **106**, 3283-3293 (2002).
52. N. Iordanova and S. Hammes-Schiffer, "Theoretical investigation of large kinetic isotope effects for proton-coupled electron transfer in ruthenium polypyridyl complexes," *J. Am. Chem. Soc.* **124**, 4848-4856 (2002).
53. C. Carra, N. Iordanova, and S. Hammes-Schiffer, "Proton-coupled electron transfer in DNA-acrylamide complexes," *J. Phys. Chem. B* **106**, 8415-8421 (2002).
54. S. P. Webb, T. Iordanov, and S. Hammes-Schiffer, "Multiconfigurational nuclear-electronic orbital approach: Incorporation of nuclear quantum effects in electronic structure calculations," *J. Chem. Phys.* **117**, 4106-4118 (2002).
55. S. Hammes-Schiffer, "Impact of enzyme motion on activity," *Biochemistry* **41**, 13335-13343 (2002).
56. J. B. Watney, P. K. Agarwal, and S. Hammes-Schiffer, "Effect of mutation on enzyme motion in dihydrofolate reductase," *J. Am. Chem. Soc.* **125**, 3745-3750 (2003).
57. T. Iordanov and S. Hammes-Schiffer, "Vibrational analysis for the nuclear-electronic orbital method," *J. Chem. Phys.* **118**, 9489-9496 (2003).
58. S. J. Benkovic and S. Hammes-Schiffer, "A perspective on enzyme catalysis," *Science* **301**, 1196-1202 (2003).

59. S. Y. Kim and S. Hammes-Schiffer, "Molecular dynamics with quantum transitions for proton transfer: Quantum treatment of hydrogen and donor-acceptor motions," *J. Chem. Phys.* **119**, 4389-4398 (2003).
60. C. Carra, N. Iordanova, and S. Hammes-Schiffer, "Proton-coupled electron transfer in a model for tyrosine oxidation in photosystem II," *J. Am. Chem. Soc.* **125**, 10429-10436 (2003).
61. S. Hammes-Schiffer and N. Iordanova, "Theoretical studies of proton-coupled electron transfer reactions," *Biochim. Biophys. Acta* **1655**, 29-36 (2004).
62. M. V. Pak and S. Hammes-Schiffer, "Electron-proton correlation for hydrogen tunneling systems," *Phys. Rev. Lett.* **92**, 103002 (2004).
63. S. Hammes-Schiffer, "Quantum-classical simulation methods for hydrogen transfer in enzymes: A case study of dihydrofolate reductase," *Curr. Opin. Struct. Biol.* **14**, 192-201 (2004).
64. E. Hatcher, A. V. Soudackov, and S. Hammes-Schiffer, "Proton-coupled electron transfer in soybean lipoxygenase," *J. Am. Chem. Soc.* **126**, 5763-5775 (2004).
65. O. Vendrell, M. Moreno, J. M. Lluch, and S. Hammes-Schiffer, "Molecular dynamics of excited state intramolecular proton transfer: 2-(2'-hydroxyphenyl)-4-methyloxazole in gas phase, solution and protein environments," *J. Phys. Chem. B* **108**, 6616-6623 (2004).
66. M. V. Pak, C. Swalina, S. P. Webb, and S. Hammes-Schiffer, "Application of the nuclear-electronic orbital method to hydrogen transfer systems: Multiple centers and multiconfigurational wavefunctions," *Chemical Physics* **304**, 227-236 (2004).
67. K. F. Wong, J. B. Watney, and S. Hammes-Schiffer, "Analysis of electrostatics and correlated motions for hydride transfer in dihydrofolate reductase," *J. Phys. Chem. B* **108**, 12231-12241 (2004).
68. S. Hammes-Schiffer, "Kinetic isotope effects for proton-coupled electron transfer reactions," pp. 499-519 in *Isotope Effects in Chemistry and Biology*, eds. H. Limbach and A. Kohen (CRC Press, Taylor & Francis Group, LLC, Boca Raton, 2005).
69. A. Soudackov, E. Hatcher, and S. Hammes-Schiffer, "Quantum and dynamical effects of proton donor-acceptor vibrational motion in nonadiabatic proton-coupled electron transfer reactions," *J. Chem. Phys.* **122**, 014505 (2005).
70. C. Swalina, M. V. Pak, and S. Hammes-Schiffer, "Alternative formulation of many-body perturbation theory for electron-proton correlation," *Chem. Phys. Lett.* **404**, 394-399 (2005).
71. K. F. Wong, T. Selzer, S. J. Benkovic, and S. Hammes-Schiffer, "Impact of distal mutations on the network of coupled motions correlated to hydride transfer in dihydrofolate reductase," *Proc. Nat. Acad. Sci. USA* **102**, 6807-6812 (2005).
72. C. Swalina, M. V. Pak, and S. Hammes-Schiffer, "Analysis of the nuclear-electronic orbital method for model hydrogen transfer systems," *J. Chem. Phys.* **123**, 014303 (2005).
73. A. Reyes, M. V. Pak, and S. Hammes-Schiffer, "Investigation of isotope effects with the nuclear-electronic orbital approach," *J. Chem. Phys.* **123**, 064104 (2005).
74. E. Hatcher, A. Soudackov, and S. Hammes-Schiffer, "Nonadiabatic proton-coupled electron transfer reactions: Impact of donor-acceptor vibrations, reorganization energies, and couplings on dynamics and rates," *J. Phys. Chem. B* **109**, 18565-18574 (2005).
75. J. H. Skone, M. V. Pak, and S. Hammes-Schiffer, "Nuclear-electronic orbital nonorthogonal configuration interaction approach," *J. Chem. Phys.* **123**, 134108 (2005).
Erratum: *J. Chem. Phys.* **128**, 229903 (2008).
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115. I. Navrotskaya and S. Hammes-Schiffer, "Electrochemical proton-coupled electron transfer: Beyond the golden rule," *J. Chem. Phys.* **131**, 024112 (2009).

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117. A. Chakraborty, M. V. Pak, and S. Hammes-Schiffer, "Properties of the exact universal functional in multicomponent density functional theory," *J. Chem. Phys.* **131**, 124115 (2009).
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119. S. J. Edwards, A. V. Soudackov, and S. Hammes-Schiffer, "Driving force dependence of rates for nonadiabatic proton and proton-coupled electron transfer: Conditions for inverted region behavior," *J. Phys. Chem. B* (in press).
120. B. Auer, M. V. Pak, and S. Hammes-Schiffer, "Nuclear-electronic orbital method within the fragment molecular orbital approach," *J. Phys. Chem. C* (in press).
121. D. K. Charavorty, A. V. Soudackov, and S. Hammes-Schiffer, "Hybrid quantum/classical molecular dynamics simulations of the proton transfer reactions catalyzed by ketosteroid isomerase: Analysis of hydrogen bonding, conformational motions, and electrostatics," *Biochemistry* (in press).
122. C. Venkataraman, A. V. Soudackov, and S. Hammes-Schiffer, "Dynamics of photoinduced proton-coupled electron transfer at molecule-semiconductor interfaces: A reduced density approach," *J. Phys. Chem. C* (submitted).

Invited Talks and Seminars

1. University of Maryland (physical chemistry seminar), College Park, Maryland, April, 1995: "Including Quantum Effects in the Simulation of Proton Transfer: How the Hydrogen Hops"
2. American Chemical Society National Meeting, Symposium on Proton transfer, Chicago, Illinois, August 21-24, 1995 (invited talk): "Proton Transfer in Solution: Molecular Dynamics with Quantum Transitions"
3. University of Notre Dame (biochemistry seminar), Notre Dame, Indiana, January 10, 1996 (invited talk): "Including Quantum Effects in the Simulation of Proton Transfer: How the Hydrogen Hops"
4. Gordon Research Conference on Isotopes in Biology and Chemistry, Ventura, California, February 11-16, 1996 (invited talk): "Including Quantum Effects in the Simulation of Proton Transfer: How the Hydrogen Hops"
5. Midwest Theoretical Chemistry Conference, Indianapolis, Indiana, May 30-June 1, 1996 (talk): "Multiconfigurational Molecular Dynamics with Quantum Transitions: Multiple Proton Transfer Reactions"
6. Telluride Workshop on Structure and Dynamics of Biophysical and Condensed Matter Systems, Telluride, Colorado, July 14-20, 1996 (invited talk): "Multiconfigurational Molecular Dynamics with Quantum Transitions"
7. Mesilla Workshop on Comparison of Classical and Quantum Dynamics, Mesilla, New Mexico, February 9-12, 1997 (invited talk): "Proton, Hydride, and Electron Transfer Reactions in Solution"
8. University of Toledo (departmental seminar), Toledo, Ohio, May 14, 1997: "Simulation of Biologically Important Charge Transfer Reactions"
9. International Discussion Meeting on Hydrogen Transfer: Experiment and Theory, Berlin, Germany, September 9-13, 1997 (invited talk): "Simulation of Multiple Proton and Hydride Transfer Reactions in Solution"
10. Michigan State University (physical chemistry seminar), East Lansing, Michigan, October 21, 1997: "Simulation of Biologically Important Charge Transfer Reactions"
11. Rice University (departmental seminar), Houston, Texas, April 14, 1998: "Simulation of Biologically Important Charge Transfer Reactions"
12. Wayne State University (physical chemistry seminar), Detroit, Michigan, April 22, 1998: "Simulation of Biologically Important Charge Transfer Reactions"
13. CECAM workshop on Combined Quantum Mechanical-Classical Hybrid Methods for the Simulation of Chemical Reactions, Lyon, France, May 26-29, 1998 (invited talk): "Mixed Quantum/Classical Molecular Dynamics with Multiple Vibrational Quantum Modes"
14. Faraday Discussion on Chemical Reaction Theory, Edinburgh, Scotland, July 1-3, 1998 (presented paper): "Quantum Dynamics of Multiple Modes for Reactions in Complex Systems"
15. Telluride Workshop on Condensed Phase Dynamics, Telluride, Colorado, July 19-25, 1998 (invited talk): "Mixed Quantum/Classical Molecular Dynamics with Multiple Vibrational Quantum Modes and Mixed Electronic/Vibrational States"
16. American Chemical Society National Meeting, Symposium on Proton-Coupled Electron Transfer, Boston, Massachusetts, August 25, 1998 (invited talk): "Theory of Proton-Coupled Electron Transfer"
17. University of North Carolina (physical chemistry seminar), Chapel Hill, North Carolina, September 3, 1998: "Simulation of Multiple Proton Transfer and Proton-Coupled Electron Transfer Reactions"
18. Duke University (departmental seminar), Durham, North Carolina, September 4, 1998: "Simulation of Multiple Proton Transfer and Proton-Coupled Electron Transfer Reactions"
19. CECAM workshop on Computational Methods for Studying the Dynamics of Quantum Systems, Lyon, France, September 28-October 1, 1998 (invited talk): "Mixed Quantum/Classical Molecular Dynamics with Multiple Vibrational Quantum Modes and Mixed Electronic/Vibrational States"

20. Iowa State University (departmental seminar), Ames, Iowa, November 5, 1998: "Simulation of Multiple Proton Transfer and Proton-Coupled Electron Transfer Reactions"
21. University of Southern Illinois (departmental seminar), Carbondale, Illinois, December 4, 1998: "Simulation of Multiple Proton Transfer and Proton-Coupled Electron Transfer Reactions"
22. Sanibel Symposium, St. Augustine, Florida, February 27-March 5, 1999 (invited talk): "Multiple Proton Transfer and Proton-Coupled Electron Transfer Reactions"
23. Henry Eyring Workshop on Time-Dependent Quantum Molecular Dynamics, Brian Head, Utah, March 13-17, 1999 (invited talk): "Multistate Continuum Theory and Nonadiabatic Dynamics for Multiple Charge Transfer Reactions"
24. AFOSR HEDM Contractor's Conference, Cocoa Beach, Florida, June 8-11, 1999 (invited talk): "Nonadiabatic Dynamics of Photoexcited Reactions and Solvation Effects for Fundamental Organic Reactions"
25. American Conference on Theoretical Chemistry, Boulder, Colorado, June 27-July 2, 1999 (invited talk): "Multiple Charge Transfer Reactions in the Condensed Phase"
26. Emory University (seminar), Atlanta, Georgia, July 15, 1999: "Multiple Charge Transfer Reactions: Physical Chemistry in Biological Systems"
27. Conference on the Dynamics of Molecular Collisions, Split Rock, Pennsylvania, July 18-23, 1999 (invited talk): "Nonadiabatic Dynamics of Charge Transfer Reactions"
28. American Chemical Society National Meeting, Symposium on Nonadiabatic Processes, New Orleans, Louisiana, August 23-27, 1999 (talk): "Proton-Coupled Electron Transfer Reactions in Solution"
29. American Chemical Society National Meeting, Symposium on QM/MM Methods, New Orleans, Louisiana, August 23-27, 1999 (invited talk): "Nonadiabatic Molecular Dynamics of Charge Transfer Reactions"
30. University of Notre Dame (physical chemistry seminar), Notre Dame, Indiana, September 2, 1999 (invited talk): "Multiple Charge Transfer Reactions: Physical Chemistry in Biological Systems"
31. Cornell University, Ithaca, New York, September 16, 1999 (departmental colloquium): "Multiple Charge Transfer Reactions: Physical Chemistry in Biological Systems"
32. Syracuse University, Syracuse, New York, September 17, 1999 (departmental colloquium): "Multiple Charge Transfer Reactions: Physical Chemistry in Biological Systems"
33. Colorado State University, Fort Collins, Colorado, October 7, 1999 (physical chemistry seminar): "Multiple Charge Transfer Reactions: Physical Chemistry in Biological Systems"
34. University of Colorado, Boulder, Colorado, October 8, 1999 (physical chemistry seminar): "Multiple Charge Transfer Reactions: Physical Chemistry in Biological Systems"
35. Penn State University, University Park, Pennsylvania, October 21, 1999 (departmental colloquium): "Multiple Charge Transfer Reactions: Physical Chemistry in Biological Systems"
36. University of Illinois, Urbana, Illinois, October 27, 1999 (physical chemistry seminar): "Multiple Charge Transfer Reactions: Physical Chemistry in Biological Systems"
37. Gordon Research Conference on Metals in Biology, Ventura, California, January 23-27, 2000 (invited talk): "Theoretical Perspectives on Proton-Coupled Electron Transfer"
38. University of California, Davis, California, January 27, 2000 (physical chemistry seminar): "Multiple Charge Transfer Reactions: Physical Chemistry in Biological Systems"
39. American Physical Society National Meeting, Symposium on Experimental and Theoretical Frontiers in Molecular Quantum Dynamics, Minneapolis, Minnesota, March 20-24, 2000 (invited talk): "Theoretical Formulation of Proton-Coupled Electron Transfer Reactions in Solution"
40. American Chemical Society New Jersey Section Meeting, Princeton, New Jersey, May 23, 2000 (invited talk): "Theoretical Perspectives on Proton-Coupled Electron Transfer"

41. Gordon Research Conference on Photosynthesis, Meriden, New Hampshire, June 18-23, 2000 (invited talk): "Theoretical Perspectives on Proton-Coupled Electron Transfer"
42. Reaction Mechanisms Conference, Madison, Wisconsin, June 24-29, 2000 (invited talk): "Theoretical Perspectives on Proton-Coupled Electron Transfer"
43. Canadian Computational Chemistry Conference, Quebec, Canada, July 30-August 3, 2000 (invited talk): "Theoretical Perspectives on Proton-Coupled Electron Transfer"
44. American Chemical Society National Meeting, Washington D.C., August 20-24, 2000 (invited talk): "Theoretical Perspectives on Proton-Coupled Electron Transfer"
45. International Workshop on Methods for Macromolecular Modeling, New York, New York, October 12-14, 2000 (invited talk): "Mixed Quantum/Classical Molecular Dynamics Simulation of Proton and Hydride Transfer Reactions in Enzymes"
46. Northwestern University, Evanston, Illinois, December 5, 2000 (physical chemistry seminar): "Proton, Hydride, and Proton-Coupled Electron Transfer Reactions in Solution and Enzymes"
47. University of Wisconsin, Madison, Wisconsin, March 20, 2001 (physical chemistry seminar): "Theoretical Perspectives of Proton-Coupled Electron Transfer"
48. AFOSR Molecular Dynamics and Theoretical Chemistry Contractor's Meeting, Irvine, California, May 21-23, 2001 (invited talk): "Nuclear Quantum Effects in Hydrogen Transfer Reactions for the Synthesis of Polyhedral Oligomeric Silsesquioxanes"
49. CECAM Workshop on New Methods for Combining Born-Oppenheimer Ab Initio Calculations and Empirical Forcefields in Large Scale Simulation Studies, Lyon, France, June 11-13, 2001 (invited talk): "Hybrid Approach for Including Electronic and Nuclear Quantum Effects in the Dynamical Simulation of Hydrogen Transfer in Enzymes"
50. Gordon Research Conference on Enzymes, Coenzymes, and Metabolic Pathways, Meriden, New Hampshire, July 22-26, 2001 (invited talk): "Molecular dynamics studies of the relation between enzyme motion and activity"
51. American Chemical Society National Meeting, Symposium on First Principles Simulation of Chemical Dynamics, Chicago, Illinois, August 26-30, 2001 (talk): "Incorporating Electronic and Nuclear Quantum Effects in the Dynamical Simulation of Proton and Hydride Transfer"
52. American Chemical Society National Meeting, Symposium on Three-Dimensional Silicon-Oxygen Cages: Materials for the 21st Century, Chicago, Illinois, August 26-30, 2001 (invited talk): "Nuclear Quantum Effects in Hydrogen Transfer Reactions for the Synthesis of Polyhedral Oligomeric Silsesquioxanes"
53. American Chemical Society National Meeting, Symposium on Hybrid QM/MM Methods for Large Molecular Systems, Chicago, Illinois, August 26-30, 2001 (invited talk): "Hybrid Approach for Simulating the Dynamics of Proton and Hydride Transfer in Enzymes"
54. Temple University, Philadelphia, Pennsylvania, October 18, 2001 (departmental colloquium): "Molecular Dynamics Studies of the Relation between Enzyme Motion and Activity"
55. Symposium on Structure and Mechanism in Biological Pathways, University Park, Pennsylvania, October 20, 2001 (invited talk): "Molecular Dynamics Studies of the Relation between Enzyme Motion and Activity"
56. Pennsylvania State University, University Park, Pennsylvania, February 15, 2002 (chemical physical seminar): "Molecular Dynamics Studies of the Relation between Enzyme Motion and Activity"
57. Maria Goeppert Mayer Interdisciplinary Symposium, San Diego, California, March 2, 2002 (keynote speaker): "Molecular Dynamics Studies of the Relation between Enzyme Motion and Activity"
58. American Chemical Society National Meeting, Symposium on Structure-Function Correlation in Enzyme Action, Orlando, Florida, April 7-11, 2002 (invited talk): "Molecular Dynamics Studies of the Relation between Enzyme Motion and Activity"

59. American Chemical Society National Meeting, Symposium on Tools for Exploring Potential Energy Surfaces, Orlando, Florida, April 7-11, 2002 (invited talk): "Multiconfigurational Nuclear-Electronic Orbital (NEO) Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"
60. International Workshop on Quantum Dynamical Concepts: From Diatomics to Biomolecules, Dresden, Germany, April 15-19, 2002 (invited talk): "Hybrid Quantum-Classical Molecular Dynamics of Hydrogen Transfer Reactions"
61. CECAM workshop on Methods for Computer Simulation of Nonadiabatic Charge Transfer Processes in the Condensed Phase, Lyon, France, April 22-24, 2002 (invited talk): "Multiconfigurational Nuclear-Electronic Orbital (NEO) Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"
62. Great Lakes Regional Meeting of the American Chemical Society, Symposium on Computational Biology, Minneapolis, Minnesota, June 2-4, 2002 (invited talk): "Hybrid Quantum-Classical Molecular Dynamics Studies of the Relation between Enzyme Motion and Activity"
63. Reaction Mechanism Conference, Columbus, Ohio, June 29-July 2, 2002 (invited talk): "Molecular Dynamics Studies of the Relation between Enzyme Motion and Activity"
64. Gordon Research Conference on Computational Chemistry, New London, New Hampshire, June 30-July 5, 2002 (invited talk): "Hybrid Quantum-Classical Molecular Dynamics of Proton and Hydride Transfer Reactions in Enzymes"
65. Workshop on Condensed Phase Dynamics, Telluride, Colorado, July 22-26, 2002 (invited talk): "Multiconfigurational Nuclear-Electronic Orbital (NEO) Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"
66. Public Lecture, Telluride, Colorado, July 25, 2002 (invited talk): "How Do Biological Enzymes Work?"
67. National American Chemical Society Meeting, Symposium on Classical and Quantum Statistical Mechanics Studies of Solvation, Boston, Massachusetts, August 18-22, 2002 (invited talk): "Theoretical Studies of Proton-Coupled Electron Transfer Reactions in Solution"
68. Rutgers University, Newark, New Jersey, September 13, 2002 (seminar): "Theoretical Perspectives of Proton-Coupled Electron Transfer Reactions"
69. University of California at Berkeley, Berkeley, California, November 12, 2002 (physical chemistry seminar): "Theoretical Perspectives of Proton-Coupled Electron Transfer"
70. Stanford University, Stanford, California, November 13, 2002 (seminar): "Hybrid Quantum-Classical Molecular Dynamics Studies of the Relation between Enzyme Motion and Activity"
71. CIMMS/CALTECH Workshop entitled Molecular Modeling and Computation: Perspectives and Challenges, Caltech, Pasadena, California, November 15-16, 2002 (invited talk): "Hybrid Quantum-Classical Molecular Dynamics of Hydrogen Transfer Reactions in Enzymes"
72. Columbia University, New York, New York, January 31, 2003 (biophysics seminar): "The Impact of Enzyme Motion on Activity"
73. Sanibel Symposium, St. Augustine, Florida, February 22-March 1, 2003 (invited talk): "Hybrid Quantum-Classical Molecular Dynamics of Hydrogen Transfer Reactions in Enzymes"
74. American Chemical Society National Meeting, Symposium on New Electronic Structure Methods: From Molecules to Materials, New Orleans, Louisiana, March 22-26, 2003 (invited talk): "Incorporation of Nuclear Quantum Effects in Electronic Structure Calculations: Multiconfigurational Nuclear-Electronic Orbital Method"
75. American Chemical Society National Meeting, Symposium on Integrating Diverse Computational Approaches to Complex Problem Solving, New Orleans, Louisiana, March 22-26, 2003 (invited talk): "Hybrid Quantum-Classical Molecular Dynamics of Hydrogen Transfer Reactions in Enzymes"

76. American Chemical Society National Meeting, Symposium on The Cutting Edge: Use of Computers in Teaching and Learning Chemistry, New Orleans, Louisiana, March 22-26, 2003 (invited talk): "Utilization of Computer Movies to Illustrate Quantum Effects and Motion in Enzyme Reactions"
77. American Society of Biochemistry and Molecular Biology National Meeting, Session on Fundamental and Emerging Issues in Enzymatic Catalysis, San Diego, California, April 12-16, 2003 (invited talk): "Impact of Enzyme Motion on Activity"
78. AFOSR Molecular Dynamics Contractor's Meeting, San Diego, California, May 18-20, 2003 (invited talk): "Nuclear Quantum Effects in Hydrogen Transfer Reactions: Polyhedral Oligomeric Silsesquioxanes and Ionic Liquids"
79. Gordon Research Conference on Photosynthesis, New Hampshire, June 22-26, 2003 (invited talk): "Coupling of Electrons and Protons to the Environment"
80. Workshop entitled Radicals in the Rockies, Telluride, Colorado, July 6-12, 2003 (invited talk): "Proton-Coupled Electron Transfer in Solution and Enzymes"
81. International meeting entitled Multidimensional Quantum Reaction Dynamics, Freie Universitat, Berlin, Germany, July 16-18, 2003 (invited talk): "Hybrid Quantum-Classical Calculations of Hydrogen Transfer Reactions"
82. Symposium entitled Computational Modelling of Catalysis, Max Planck Institute, Muelheim, Germany, July 16-18, 2003 (invited talk): "Hybrid Quantum-Classical Molecular Dynamics of Hydrogen Transfer Reactions in Enzymes"
83. Conference entitled Excited State Processes in Electronic and Bio Nanomaterials, Los Alamos, New Mexico, August 11-16, 2003 (invited talk): "Proton-Coupled Electron Transfer Reactions"
84. American Chemical Society National Meeting, Symposium on Making and Breaking Chemical Bonds in Gas and Condensed Phases: Theory and Applications, New York, New York, September 7-11, 2003 (invited talk): "Investigation of Hydrogen Transfer Reactions with the Multiconfigurational Nuclear-Electronic Orbital Method"
85. Central Regional American Chemical Society Meeting, Pittsburgh, Pennsylvania, October 19-23, 2003 (invited talk): "Hybrid Quantum-Classical Molecular Dynamics of Hydrogen Transfer Reactions in Enzymes"
86. University of Iowa, Iowa City, Iowa, November 6, 2003 (colloquium): "Impact of Enzyme Motion on Activity"
87. Indiana University, Bloomington, Indiana, February 5, 2004 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
88. Gordon Research Conference on Isotopes in Biological and Chemical Sciences, Ventura, California, February 14-20, 2004 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
89. American Physical Society National Meeting, Montreal, Canada, March 22-26, 2004 (invited talk): "Hybrid Quantum-Classical Molecular Dynamics of Hydrogen Transfer Reactions in Enzymes"
90. American Chemical Society National Meeting, Symposium on Mixed Quantum, Classical and Semiclassical Dynamics, Anaheim, California, March 28-April 1, 2004 (invited talk): "Electron-Proton Correlation in the Nuclear-Electronic Orbital Method: Applications to Hydrogen Tunneling Systems"
91. NSF-UK N+N meeting, Washington, D.C., April 15-16, 2004 (invited talk): "Hybrid Quantum-Classical Molecular Dynamics of Enzyme Reactions"
92. University of Minnesota, Minneapolis, Minnesota, April 23, 2004 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
93. Johns Hopkins University, Baltimore, Maryland, May 4, 2004 (Ephraim and Wilma Shaw Roseman Lecturer): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
94. Canadian Society for Chemistry Conference, London, Ontario, May 29-June 1, 2004 (invited talk): "Hybrid Quantum-Classical Molecular Dynamics of Hydrogen Transfer Reactions in Enzymes"

95. Workshop on Condensed Phase Dynamics, Telluride, Colorado, July 19-23, 2004 (invited talk): "Proton-Coupled Electron Transfer"
96. MERCURY Undergraduate Research Conference, Hamilton College, July 29-31, 2004 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
97. Protein Society Annual Symposium, San Diego, California, August 15, 2004 (invited talk): "Utilization of Computational Approaches to Elucidate Enzyme Mechanisms"
98. Yale University, New Haven, Connecticut, September 14, 2004 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
99. Colorado State University, Fort Collins, Colorado, October 14, 2004 (physical chemistry seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
100. University of Colorado, Boulder, Colorado, October 15, 2004 (physical chemistry seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
101. University of Massachusetts at Amherst, Amherst, Massachusetts, November 16, 2004 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
102. Mount Holyoke College, November 17, 2004, Lucy Pickett Lecturer: "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
103. McGill University, Montreal, Canada, November 23, 2004, Donald Lecturer: "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
104. Harvard University and Massachusetts Institute of Technology, Boston, Massachusetts, December 9, 2004 (Woodward Lecture Series, Harvard/MIT physical chemistry seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
105. 19th Enzyme Mechanisms Conference, Pacific Grove, California, January 5-9, 2005 (invited talk): "Impact of Enzyme Motion on Activity"
106. Gordon Research Conference on Molecular Energy Transfer, Buellton, California, January 9-15, 2005 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
107. American Chemical Society National Meeting, Symposium on Hydrogen Bonds: Developments in Experiment and Theory, San Diego, California, March 13-17, 2005 (invited talk): "Impact of Nuclear Quantum Effects on Hydrogen Bonding and Proton Transfer Reactions"
108. Princeton University, Princeton, New Jersey, March 31, 2005 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
109. Duke University, Durham, North Carolina, April 5, 2005 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
110. University of Toronto, Chemical Biophysics Symposium, April 8-10, 2005 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
111. University of Michigan, Ann Arbor, Michigan, April 21, 2005 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
112. Texas A&M University, College Station, Texas, May 5, 2005 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
113. Mathematical Biosciences Institute, Workshop on Enzyme Dynamics, Ohio State University, May 19-21, 2005 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
114. AFOSR Contractor's Meeting, Monterey, California, May 22-25, 2005 (invited talk): "Impact of Nuclear Quantum Effects on Hydrogen Bonding and Proton Transfer Reactions"
115. American Conference on Theoretical Chemistry, Los Angeles, California, July 16-21, 2005 (invited talk): "Proton-Coupled Electron Transfer: Analysis of Dynamics and Calculations of Couplings"
116. American Chemical Society National Meeting, Symposium on Electron Transfer Processes: Making Connections, Washington, D.C., August 28-September 1, 2005 (invited talk): "Proton-Coupled Electron Transfer Reactions in Solution and Proteins"

117. American Chemical Society National Meeting, Symposium on Theoretical Determination of Energy Landscapes: Methodology and Applications, Washington, D.C., August 28-September 1, 2005 (invited talk): “Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations”
118. University of Houston, Houston, Texas, September 14, 2005 (seminar): “Hydrogen Tunneling and Protein Motion in Enzyme Reactions”
119. University of Texas at Austin, Austin, Texas, September 15, 2005 (seminar): “Hydrogen Tunneling and Protein Motion in Enzyme Reactions”
120. Baker Symposium, Cornell University, Ithaca New York, October 1, 2005 (invited talk): “Hydrogen Tunneling and Protein Motion in Enzyme Reactions”
121. University of Maryland, College Park, Maryland, October 5, 2005 (seminar): “Hydrogen Tunneling and Protein Motion in Enzyme Reactions”
122. Royal Society Discussion Meeting on Quantum Catalysis in Enzymes – Beyond the Transition State Theory Paradigm, London, November 14-15, 2005 (invited talk) “Hydrogen Tunneling and Protein Motion in Enzyme Reactions”
November 16, 2005: Chair the Novartis Foundation Royal Society Discussion Meeting on “Computational Approaches to H-Transfer”
123. Pacifichem Conference, Symposium on Nonadiabatic Phenomena and Related Dynamics: Theory and Experiment, Honolulu, Hawaii, December 15-20, 2005 (invited talk): “Nonadiabatic Proton-Coupled Electron Transfer Reactions in Solution and Proteins”
124. Pacifichem Conference, Symposium on Proton Transfer/Transport: H-bonded Solids, Liquids, Clusters, and Interfaces, Honolulu, Hawaii, December 15-20, 2005 (invited talk): “Hybrid Quantum-Classical Molecular Dynamics of Hydrogen Transfer Reactions in Enzymes”
125. Gordon Research Conference on Metals in Biology, Ventura, California, January 29-February 2, 2006 (invited talk): “Proton-Coupled Electron Transfer Reactions in Solution and Proteins”
126. Biophysical Society Annual Meeting, Salt Lake City, Utah, February 18-22, 2006 (invited talk): “Impact of Enzyme Motion on Activity”
127. American Chemical Society National Meeting, Symposium on Quantum Molecular Dynamics in the Condensed Phase: Towards Bridging the Gap between Theory and Experiment, Atlanta, Georgia, March 26-30, 2006 (invited talk): “Proton-Coupled Electron Transfer and Hydrogen Atom Transfer in the Condensed Phase”
128. Argonne National Laboratory, Argonne, Illinois, April 10, 2006 (seminar): “Hydrogen Tunneling and Protein Motion in Enzyme Reactions”
129. University of Texas Southwestern Medical Center, Dallas, Texas, April 13, 2006 (seminar): “Impact of Enzyme Motion on Activity”
130. DARPA Protein Design Processes Program Review, Islamorada, Florida, April 18-20, 2006 (invited talk): “Ranking Protein Designs According to Chemical Reaction Barriers”
131. New York University, New York, New York, April 28, 2006 (colloquium): “Hydrogen Tunneling and Protein Motion in Enzyme Reactions”
132. Oak Ridge National Laboratory, Oak Ridge, Tennessee, May 10, 2006 (seminar): “Proton-Coupled Electron Transfer Reactions in Solution and Proteins”
133. 12th International Congress of Quantum Chemistry (ICQC), Kyoto, Japan, May 21-26, 2006 (invited talk): “Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations”
134. ICQC satellite meeting on Reactions in Solution and Biological Systems: Potential Energy Surface and Dynamics, Kyoto, Japan, May 27-29, 2006 (invited talk): “Hydrogen Tunneling and Protein Motion in Enzyme Reactions”

135. Gordon Research Conference on Vibrational Spectroscopy: Probing Structure and Dynamics, Biddeford, Maine, July 2-7, 2006 (invited talk): "Proton-Coupled Electron Transfer Reactions in Solution and Proteins"
136. Gordon Research Conference on Atomic and Molecular Interactions, New London, New Hampshire, July 9-14, 2006 (invited talk): "Nuclear-Electronic Orbital Approach: Calculation of Structures, Frequencies, and Couplings"
137. Telluride Workshop on Condensed Phase Dynamics, Telluride, Colorado, July 17-23, 2006 (invited talk): "Nuclear-Electronic Orbital Approach: Calculation of Structures, Frequencies, and Couplings"
138. American Chemical Society National Meeting, Symposium entitled Beyond Michael Dewar's Legacy: Modern Semiempirical MO Theory, San Francisco, California, September 10-14, 2006 (invited talk): "Impact of Enzyme Motion on Activity"
139. American Chemical Society National Meeting, Symposium entitled Fifty Years of Electron Transfer and RRKM Theories, San Francisco, California, September 10-14, 2006 (invited talk): "Proton-Coupled Electron Transfer: Couplings, Rates, and Isotope Effects"
140. Michigan State University, East Lansing, Michigan, October 6, 2006 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
141. California Institute of Technology, Pasadena, California, November 28, 2006 (invited seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
142. Berkeley Mini Stat Mech Meeting, Berkeley, California, January 12-14, 2007 (invited talk): "Proton-Coupled Electron Transfer Reactions: Dynamics and Kinetic Isotope Effects"
143. Gordon Research Conference on Electrochemistry, Ventura, California, January 14-19, 2007 (invited talk): "Proton-Coupled Electron Transfer Reactions in Solution and Proteins"
144. DARPA Control of Protein Conformations Kickoff Meeting, San Francisco, California, February 1-2, 2007 (invited talk): "Elucidation of Allosteric Mechanisms with Molecular Dynamics"
145. Gordon Research Conference on Gaseous Ions: Structures, Energetics and Reactions, Ventura, California, February 25-March 2, 2007 (invited talk): "Nuclear-Electronic Orbital Approach: Calculation of Structures, Frequencies, and Couplings"
146. American Chemical Society National Meeting, Symposium entitled Measures of Accuracy and Reliability in Molecular Simulation, Chicago, Illinois, March 25-29, 2007 (invited talk): "Hybrid Quantum-Classical Molecular Dynamics of Hydrogen Transfer Reactions in Enzymes"
147. Annual Meeting of the American Society for Biochemistry and Molecular Biology, Symposium entitled Computational Studies of Mechanistic and Dynamical Aspects of Enzyme Reactions, Washington, DC, April 28-May 2, 2007 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
148. 7th Annual Symposium of the Centre for Research in Molecular Modeling (CERMM), Montreal, Canada, May 4-6, 2007 (plenary lecture): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
149. AFOSR Contractor's Conference, Irvine, California, May 20-22, 2007 (invited talk): "Nuclear-Electronic Orbital Approach: Recent Advances and Applications"
150. Molecular Quantum Mechanics International Conference, Budapest, Hungary, May 29-June 3, 2007 (invited talk): "Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"
151. Gordon Research Conference on Molecular and Cellular Bioenergetics, Andover, New Hampshire, June 17-22, 2007 (invited talk): "Proton-Coupled Electron Transfer in Proteins: Dynamics and Kinetic Isotope Effects"
152. Midwest Theoretical Chemistry Conference, Bloomington, Indiana, June 28-30, 2007 (plenary talk): "Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"

153. CECAM workshop on Theoretical and Experimental Exploration of Quantum Dynamics in Condensed Phase Chemical Systems, Dublin, Ireland, August 7-10, 2007 (invited talk): "Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"
154. American Chemical Society National Meeting, Symposium entitled Hydration: From Clusters to Solution, Boston, Massachusetts, August 19-23, 2007 (invited talk): "Role of Water in Proton-Coupled Electron Transfer Reactions"
155. American Chemical Society National Meeting, Symposium entitled Strategies in Enzymatic Oxidation Catalysis, Boston, Massachusetts, August 19-23, 2007 (invited talk): "Proton-Coupled Electron Transfer in Soybean Lipoxygenase: Dynamical Behavior and Kinetic Isotope Effects"
156. Pittsburgh University, Pittsburgh, Pennsylvania, September 20, 2007 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
157. XIV International Workshop on Quantum Atomic and Molecular Tunneling in Solids and other Condensed Phases, Houston, Texas, October 28-November 1, 2007 (invited talk): "Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"
158. 16th Conference on Current Trends in Computational Chemistry, Jackson, Mississippi, November 2-3, 2007 (invited talk): "Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"
159. Gordon Research Conference in Biomolecular Interactions and Methods, Ventura, California, January 13-18, 2008 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
160. Wayne State University, Detroit, Michigan, March 18, 2008 (invited talk, medical school): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
161. Wayne State University, Detroit, Michigan, March 19, 2008 (invited talk, physical chemistry seminar): "Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"
162. University of California Berkeley Structural and Quantitative Biology seminar, April 21, 2008 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
163. Conference on Protein Dynamics and Catalysis, Tarrytown, New York, May 2-4, 2008 (invited talk): "Proton-Coupled Electron Transfer in Soybean Lipoxygenase: Dynamical Behavior and Kinetic Isotope Effects"
164. Central East Regional ACS Meeting, Symposium entitled Theoretical Models of Solvation: Methods and Applications, Columbus, Ohio, June 11-14, 2008 (invited talk): "Proton-Coupled Electron Transfer Reactions in Solution and at Electrochemical Interfaces"
165. 13th International Workshop on Quantum Systems in Chemistry and Physics (QSCP-XIII), Lansing, Michigan, July 6-12, 2008 (invited talk): "Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"
166. 6th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VI), Vancouver, Canada, July 19-24, 2008 (plenary talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
167. 6th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VI), Vancouver, Canada, July 19-24, 2008 (invited talk): "Hybrid Quantum/Classical Molecular Dynamics of Hydrogen Transfer Reactions in Enzymes"
168. Gordon Research Conference on Electron Donor Acceptor Interactions, Newport, Rhode Island, August 3-8, 2008 (invited talk): "Proton-Coupled Electron Transfer Reactions in Solution, Proteins, and Electrochemistry"
169. American Chemical Society National Meeting, Symposium entitled Water Mediated Interactions, Philadelphia, Pennsylvania, August 17-21, 2008 (talk): "Role of Water in Proton-Coupled Electron Transfer"

170. American Chemical Society National Meeting, Symposium entitled Biological and Biomimetic Interfacial Electron Transfer, Philadelphia, Pennsylvania, August 17-21, 2008 (invited talk): "Electrochemical Proton-Coupled Electron Transfer"
171. University of Akron, Akron, Ohio, November 11, 2008 (invited talk): "Proton-Coupled Electron Transfer in Solution, Proteins, and Electrochemistry"
172. Akron Section Award Address, Akron, Ohio, November 11, 2008 (award talk): "How do Biological Enzymes Work?"
173. Osaka University Forum 2008, San Francisco, California, December 8-11, 2008 (invited talk): "Proton-Coupled Electron Transfer in Energy Conversion"
174. Workshop on Chemical Dynamics: Challenges and Approaches for a Thematic Year in Mathematics and Chemistry at the Institute for Mathematics and its Applications at the University of Minnesota, Minneapolis, Minnesota, January 12-16, 2009 (invited talk): "Nuclear-Electronic Orbital Approach: Electron-Proton Correlation, Multicomponent Density Functional Theory, and Tunneling Splittings"
175. Gordon Research Conference on Protons and Membrane Reactions, Ventura, California, February 22-27, 2009 (invited talk): "Proton-Coupled Electron Transfer Reactions in Enzymes: Hydrogen Tunneling and Protein Motion"
176. Sanibel Symposium, St. Simons Island, Georgia, February 26- March 3, 2009 (invited talk): "Proton-Coupled Electron Transfer Reactions in Enzymes: Hydrogen Tunneling and Protein Motion"
177. American Chemical Society National Meeting, Symposium entitled Advances in Electronic Structure Theory and First Principles Dynamics, Salt Lake City, Utah, March 22-26, 2009 (invited talk): "Electron-Proton Correlation in the Nuclear-Electronic Orbital Approach: Explicit Correlation and Multicomponent Density Functional Theory"
178. American Chemical Society National Meeting, Symposium entitled Functional Motions in Enzyme Catalysis, Salt Lake City, Utah, March 22-26, 2009 (invited talk): "Proton-Coupled Electron Transfer in Soybean Lipoxxygenase: Impact of Mutation on Enzyme Motions Coupled to Catalysis"
179. Ohio State University, Columbus, Ohio, April 13, 2009 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
180. Franklin Institute, Philadelphia, Pennsylvania, April 23, 2009 (invited talk): "Impact of Enzyme Motion on Activity"
181. University of Washington, Seattle, Washington, April 29, 2009 (invited talk): "Proton-Coupled Electron Transfer in Solution, Proteins, and Electrochemistry"
182. AFOSR Contractor's Meeting, San Diego, California, May 17-19, 2009 (invited talk): "Nuclear-Electronic Orbital Approach: Electron-Proton Correlation and Multicomponent Density Functional Theory"
183. Gordon Research Conference on Biological Molecules in the Gas Phase and in Solution, Tilton, New Hampshire, July 5-9, 2009 (invited talk): "Proton and Hydrogen Transfer Reactions in Enzymes"
184. Canadian Computational Chemistry Conference, Halifax, Nova Scotia, Canada, July 20-24, 2009 (invited talk): "Nuclear-Electronic Orbital Approach: Electron-Proton Correlation and Multicomponent Density Functional Theory"
185. American Chemical Society National Meeting, Symposium entitled The Physical Chemistry of Photon to Fuel Conversion, Washington, D.C., August 16-20, 2009 (invited talk): "Proton-Coupled Electron Transfer in Energy Conversion"

Scheduled Talks and Seminars

186. Northwestern University, Evanston, Illinois, November 4, 2009 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"

187. Mesilla Chemistry Workshop on Electronic Nonadiabatic Dynamics, Mesilla, New Mexico, February 7-10, 2010 (invited talk): "Photoinduced Proton-Coupled Electron Transfer Reactions in Solution and at Interfaces"
188. Rice University, Houston, Texas, February 15, 2010 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
189. Gordon Research Conference on Isotopes in Biological and Chemical Sciences, Galveston, Texas, February 14-19, 2010 (invited talk): "Unusual Kinetic Isotope Effects in Proton-Coupled Electron Transfer Reactions"
190. Center for Scientific Computation and Mathematical Modeling Workshop on Quantum-Classical Modeling of Chemical Phenomenon, College Park, Maryland, March 8-11, 2010 (invited talk)
191. American Chemical Society National Meeting, Symposium entitled Computers in Chemistry, San Francisco, California, March 21-25, 2010 (invited talk): Hydrogen Bonding, Electrostatics, and Conformational Motions in Enzyme Catalysis
192. Purdue University, Department of Physics, "Biophysical, Physical Bioinorganic and Bionanotechnology" seminar series, West Lafayette, Indiana, April 13, 2010 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
193. University of South Carolina, Columbia, South Carolina, April 16, 2010 (Davis lecture): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
194. Gordon Research Conference on Enzymes, Coenzymes, and Metabolic Pathways, Waterville Valley, New Hampshire, July 18-23, 2010 (invited talk)
195. Gordon Research Conference on Atomic and Molecular Interactions, New London, New Hampshire, July 18-23, 2010 (invited talk)
196. 61st Annual Meeting of International Society of Electrochemistry, Nice, France, September 26-October 1, 2010 (invited Key-Note Lecture)

Teaching

University of Notre Dame

Chem 647: Computer Simulation of Organic and Biological Systems
Fall 1995, Fall 1996, Fall 1997

Chem 643: Seminar in Physical Chemistry
Fall 1996, Spring 1997, and Fall 1997

Chem 649: Quantum Mechanics
Spring 1997, Spring 1998

Chem 321: Physical Chemistry I (undergraduate thermodynamics and kinetics)
Fall 1999

Chem 322: Physical Chemistry II (undergraduate quantum mechanics)
Spring 2000

Penn State University

Chem 454/565: Introduction to Quantum Chemistry/Quantum Chemistry I
(advanced undergraduate and graduate quantum mechanics)
Fall 2000, 2002, 2003, 2004, 2005

Chem 452: Physical Chemistry II (undergraduate quantum mechanics and kinetics)
Fall 2001

Chem 451: Physical Chemistry I (undergraduate thermodynamics)
Fall 2006

Chem 450: Physical Chemistry I (undergraduate thermodynamics)
Fall 2007

Chem 464: Chemical Kinetics and Dynamics (advanced undergraduate course)
Fall 2009

University Service

Graduate Counseling Committee (2000-2001)
Graduate Student Admissions Committee (2000-2001)
Chair of Faculty Search Committee (2001-2002)
Graduate Counseling and Awards Committee (2002- 2004)
Chair of Department Head Search Committee (2003-2004)
Chair of Faculty Search Committee (2004-2005)
Faculty Search Committee (2005-2007)
Departmental Budget Committee (2005-2006)
Faculty Think Tank Committee (2005-2007)
Department Head Search Committee (2007)
Colloquium Committee (2000-2002, 2006-present)
Chair of Colloquium Committee (2001-2002, 2007-2008)
Departmental Promotion and Tenure Committee (2001-2005, 2006-present)
College Promotion and Tenure Committee (2006-2008)
Chair of Departmental Promotion and Tenure Committee (2007-2009)
Chair of College Promotion and Tenure Committee (2007-2008)
Faculty Awards Committee (2007-present)
Chair of Faculty Awards Committee (2009-2010)
Departmental Advisory Board (2007-2009)
College IT Faculty Steering Committee (2008-2009)
College SRDP (Staff Review and Development Plan) Task Force (2008-2009)
Member of ECOS Promotion and Tenure Panel (2009)

Outreach and Education

Public Lecture, Telluride, Colorado, July 25, 2002 (invited talk): “How Do Biological Enzymes Work?”

American Chemical Society National Meeting, Symposium on The Cutting Edge: Use of Computers in Teaching and Learning Chemistry, New Orleans, Louisiana, March 22-26, 2003 (invited talk): “Utilization of Computer Movies to Illustrate Quantum Effects and Motion in Enzyme Reactions”

MERCURY Undergraduate Research Conference, Hamilton College, July 29-31, 2004 (invited talk): “Hydrogen Tunneling and Protein Motion in Enzyme Reactions”

Protein Society Annual Symposium, Educators Lunch on Teaching Protein Science: Computational Approaches to Protein Chemistry, San Diego, California, August 15, 2004 (invited talk): “Utilization of Computational Approaches to Elucidate Enzyme Mechanisms”

Iota Sigma Pi National Honor Society of Women in Chemistry 28th National Triennial Convention, Sweet Briar, Virginia, June 10, 2005 (Agnes Fay Morgan awardee invited participant): Panel Discussion on Reflections in Research and Teaching

ACS PRF Summer School on “Probing the Dynamics of Liquids and Biomolecules: Theory and Experiment,” Telluride, Colorado, July 16-21, 2006 (invited instructor): “Mixed Quantum/Classical Molecular Dynamics Methods” and “Proton-Coupled Electron Transfer Reactions in Solution and Proteins”

Designed and created a web site on proton-coupled electron transfer (PCET) reactions, which are central in a wide range of chemical and biological processes, including energy conversion processes. The web site is open to the public at <http://webpcet.chem.psu.edu>. This web site includes a list of research groups working on PCET, a list of publications on PCET, a summary of the basic theoretical concepts of PCET, and a series of Java servlets that enable the user to interactively model PCET reactions. The objective of this web site is to increase understanding in the community about the fundamental theory of PCET and to enable experimentalists in the field to model their data.

Developed the nuclear-electronic orbital (NEO) method for the inclusion of nuclear quantum effects in electronic structure calculations and incorporated this method into the public domain version of the GAMESS electronic structure package. The GAMESS program is available free of charge to the public.