

# 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

John Gamble Kirkwood Professor of Chemistry Yale University	1/18 – present
Swanlund Professor of Chemistry University of Illinois at Urbana-Champaign	8/12 – 12/17
Eberly Professor in Biotechnology Pennsylvania State University	8/06 – 8/12
Professor of Chemistry Pennsylvania State University	7/03 – 8/12
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

G. M. Kosolapoff Award from Auburn University, 2019  
Member, Connecticut Academy of Science and Engineering (CASE), 2018  
Center for Advanced Study Professor, University of Illinois Urbana-Champaign, 2017  
Senior Fellow, Canadian Institute for Advanced Research (CIFAR), 2016 – present  
Fellow, Biophysical Society, 2015  
Blue Waters Professor, 2014 – 2018  
Member, International Academy of Quantum Molecular Science, 2014  
Member, U.S. National Academy of Sciences, 2013  
Fellow, American Association for the Advancement of Science, 2013  
Member, American Academy of Arts and Sciences, 2012  
Fellow, American Chemical Society, 2011  
National Institutes of Health MERIT Award, 2011

Fellow, American Physical Society, 2010  
American Chemical Society Akron Section Award, 2008  
International Academy of Quantum Molecular Science Medal, 2005  
Iota Sigma Pi Agnes Fay Morgan Research Award, 2005  
Alexander M. Cruickshank Lecturer, Gordon Research Conferences, 2004  
National Science Foundation Creativity Extension Award, 2003  
Camille Dreyfus Teacher-Scholar Award, 1999  
Alfred P. Sloan Research Fellowship, 1998  
Ralph E. Powe Junior Faculty Enhancement Award, Oak Ridge Associated Universities, 1998  
National Science Foundation CAREER Award, 1996  
National Science Foundation Graduate Fellowship in Chemistry, 1988-91  
AT&T Bell Laboratories GRPW (Graduate Research Program for Women) Grant, 1988-92  
American Institute of Chemists Student Award, 1988  
Merck Index Award, Princeton University, 1988  
ACS Regional Scholarship Award, 1988  
William Foster Memorial Prize in Chemistry, Princeton University, 1987

## **Named Lectureships**

24<sup>th</sup> John Stauffer Lecturer in Chemistry, Stanford University, 2019  
47<sup>th</sup> John Stauffer Lecture, University of Southern California, 2019  
Kenneth S. Pitzer Lecture in Chemistry, University of California at Berkeley, 2019  
Musselman Visiting Scientist and Lecturer, Gettysburg College, 2018  
Lifson Memorial Lecture, Weizmann Institute, Israel, 2018  
Nebraska Cluster for Computational Chemistry (NC3) Award Lecture, 2018  
Löwdin Lecturer, Uppsala University, 2017  
Neckers Lecture, Southern Illinois University, 2017  
W. A. Noyes Distinguished Lecture, University of Texas at Austin, 2017  
Armstrong Lecture, Vanderbilt University, 2017  
Walter Kauzmann Lecturer, Princeton University, 2016  
Jean Dreyfus Boissevain Lectureship, University of Colorado at Denver, 2016  
Reilly Lecturer, University of Notre Dame, 2015  
G. Wilse Robinson Lecturer, Texas Tech University, 2015  
Haines Lecturer, University of South Dakota, 2014  
Watkins Visiting Professorship, Wichita State University, 2013  
H. Willard Davis Lecturer, University of South Carolina, 2010  
Ephraim and Wilma Shaw Roseman Lecturer, Johns Hopkins University, 2004  
Lucy Pickett Lecturer, Mount Holyoke College, 2004  
Donald Lecturer, McGill University, 2004  
Woodward Lecturer, Harvard University, 2004

## **Professional Service**

Editor-in-Chief, *Chemical Reviews*, 2014 – present  
Board of Reviewing Editors, *Science*, 2016 – present  
Alfred P. Sloan Research Fellowship Selection Committee, 2013 – present  
Representative of Chemistry Section (14) for Class I Membership Committee of the National Academy of Sciences, 2015, 2017  
Member of BESAC (Basic Energy Sciences Advisory Committee) for the Department of Energy, 2008 – present

Member of Scientific Advisory Board, DOE Energy Frontier Research Center: Inorganometallic Catalyst Design Center, University of Minnesota, 2014 – present

Member of Scientific Advisory Board, DOE Hub: Joint Center for Artificial Photosynthesis, 2016 – present

Chair of Committee of Visitors for the National Science Foundation (NSF) Division of Chemistry, 2016

Member of National Academy of Sciences Award in Chemical Sciences Selection Committee, 2016

Member of American Academy of Arts and Sciences Class I Section 3 Membership Panel, 2016-2017

Member of Search Committee for the National Science Foundation (NSF) Assistant Director for Mathematical and Physical Sciences, 2016

Chair of Search Committee for the Division Director of the National Science Foundation (NSF) Division of Chemistry, 2014

Chair of Committee of Visitors (COV) for the Department of Energy (DOE) to review the Chemical Sciences, Biosciences, and Geosciences Division, April 2014

Editorial Advisory Board for *The Journal of Physical Chemistry*, 2015 – present

Editorial Advisory Board for *Journal of Chemical Theory and Computation*, 2010 – present

Editorial Advisory Board for *Accounts of Chemical Research*, 2006 – present

Vice Chair/Chair of the American Conference of Theoretical Chemistry, 2014, 2017

Deputy Editor for *The Journal of Physical Chemistry B*, 2011 – 2014

Senior Editor for *The Journal of Physical Chemistry*, 2001 – 2014

Senior Editor for *The Journal of Physical Chemistry Letters*, 2009 – 2011

Vice Chair/Chair of the Physical Chemistry Division of the American Chemical Society, 2008 – 2013

Vice Chair/Chair of the Gordon Research Conference on Atomic and Molecular Interactions, 2012, 2014

Editorial Advisory Board for *The Journal of the American Chemical Society*, 2008 – 2013

Member of a Committee of Visitors (COV) for the Department of Energy (DOE) to review the Energy Frontier Research Centers and the Solar Hub, May 2013

Ad hoc member of various NIH study sections, typically once a year, 2006 – present

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 to review the Photochemistry and Radiation Research and Condensed-phase Chemical Physics programs, April 2008

Co-organized a Workshop entitled “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

Tanner Culpitt, Zachary Kall Goldsmith, Clorice Reinhardt, Patrick Schneider, David Stevens, Zhen Tao

### Current Postdoctoral Research Assistants

Kurt Brorsen, Yan Choi Lam, Pengfei Li, Yang Yang, Josh Goings, Elvira Sayfutyarova, Fabijan Pavosevic  
Alexander Soudackov (Research Assistant Professor)

### 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, Oak Ridge National Laboratory; adjunct faculty in graduate program in  
Genome Science and Technology, University of Tennessee

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

current position: Associate Professor, Georgia Southwestern University

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

current position: Associate Professor, Georgia Southwestern University

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

current position: technical support scientist, Schrodinger, Inc.

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

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

current position: computer software programmer at Westarete

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

current position: consultant, University of Maryland, Baltimore

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

current position: Associate Professor, Department of Chemistry, CUNY York

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

current position: Computational Scientist, Research Computing Center, University of Chicago

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

current position: Research Associate: Medicinal Chemistry, University of South Australia

Dhruva Chakravorty, Ph.D., Pennsylvania State University, 2010

current position: assistant professor, University of New Orleans

Sarah Hillard Edwards, Ph.D., Pennsylvania State University, 2010

current position: chemistry instructor, University of Kentucky  
Michelle Ludlow, Ph.D., Pennsylvania State University, 2010  
Narayanan Veeraghavan, Ph.D., Pennsylvania State University, 2011  
current position: Lead Programmer Scientist, Human Genome Sequencing Center,  
Baylor College of Medicine  
Laura Fernandez, Ph.D., Pennsylvania State University, 2013  
current position: Managing Editor, American Chemical Society Publishing  
Yinxi Yu, M.S., Pennsylvania State University, 2013  
current position: Kanghong Pharmaceutical, China  
Philip Hanoian, Ph.D., Pennsylvania State University, 2014  
current position: postdoc, Pennsylvania State University  
Brian Solis, Ph.D., University of Illinois at Urbana-Champaign, 2014  
current position: Managing Editor, American Institute of Physics Publishing  
Andrew Sirjoosingh, Ph.D., University of Illinois at Urbana-Champaign, 2014  
current position: postdoc, Northwestern University  
Abir Ganguly, Ph.D., University of Illinois at Urbana-Champaign, 2014  
current position: postdoc, Rutgers University  
Sixue Zhang, Ph.D., University of Illinois at Urbana-Champaign, 2016  
current position: postdoc, Southern Research Institute  
Mioy Huynh, Ph.D., University of Illinois at Urbana-Champaign, 2017  
Current position: preceptor, general chemistry, Yale University  
Aparna Harshan, Ph.D., University of Illinois at Urbana-Champaign, 2018

#### 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, University of Illinois  
Ivan Rostov, July 1999-June 2001  
current position: computational chemist, supercomputer facility, Australian National University  
Salomon Billeter, November 1999-June 2001  
current position: unknown  
Mark Kobrak, January 2000-August 2001  
current position: associate professor, CUNY Brooklyn  
Simon Webb, August 1998-December 2001  
current position: research scientist, Advanced Biomedical Computing Center, National Cancer Institute  
Claudio Carra, August 2001- June 2003  
current position: research scientist, NASA  
Kim Fay Wong, October 2001 - July 2004  
current position: computational consultant, University of Pittsburgh  
Michael Pak, August 2003 – August 2006  
current position: unknown  
Alessandro Sergi, August 2004 – March 2005  
current position: assistant professor, University of KwaZulu-Natal

Andres Reyes, July 2003 – June 2005  
current position: assistant professor, Universidad Nacional de Colombia

Qian Wang, August 2005 – August 2006  
current position: computational science graduate student, Purdue University

Yasuhito Ohta, November 2004 – November 2006  
current position: research associate, Kyoto University

Hiroshi Ishikita, November 2005 – November 2007  
current position: assistant professor, University of Tokyo

Irina Navrotskaya, January 2007 - February 2009  
current position: math graduate student, University of Pittsburgh

Arindam Chakraborty, March 1, 2006 - August 2009  
current position: associate professor, Syracuse University

Charulatha Venkataraman, August 2007 - October 2009  
current position: Institute of Mathematical Sciences, CIT Campus, Taramani, Chennai, India

Anirban Hazra, January 2007 - June 2011  
current position: assistant professor, Indian Institute of Science Education and Research Pune

Ben Auer, September 2008 - December 2011  
current position: senior software engineer, Global Modeling and Assimilation Office, NASA

Chet Swalina, November 2009 - November 2012  
current position: computer software programmer at Westarete

Chaehyuk Ko, August 2010 - July 2013  
current position: scientist at Samsung, Korea

Samantha Horvath, August 2010 - September 2013  
current position: scientist at IllinoisRocstar in Champaign, Illinois

Josh Layfield, August 2011 – August 2014  
current position: assistant professor at University of St. Thomas, Saint Paul, Minnesota

Christine Schwerdtfeger, May 2012 - December 2014  
current position: software engineer at Enova International

Melek Nihan Ucisik, August 2014 – August 2016  
current position: researcher, Baylor College of Medicine

Tao Yu, August 2014 – August 2016  
current position: assistant professor at Tennessee Tech

Puja Goyal, August 2013 – August 2017  
current position: assistant professor at SUNY Binghamton

Soumya Ghosh, January 2013 – June 2017  
current position: postdoc at University College London

Kurt Brorsen, June 2014 – July 2018  
current position: assistant professor at University of Missouri-Columbia

#### Past Undergraduate Research Assistants

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

## 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 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)	10/1/05 - 9/30/08	\$114,725 (S.H.S.)



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
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 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 Theoretical Studies of Proton-Coupled Electron Transfer Reactions	7/1/08 - 6/30/11	\$440,000
National Science Foundation Powering the Planet: A Chemical Bonding Center in the Direct Conversion of Sunlight into Chemical Fuel (CCI group proposal, P.I. Harry Gray)	8/1/08 - 7/31/13	\$880,930 (S.H.S.)
National Science Foundation Theoretical Studies of Proton-Coupled Electron Transfer Reactions	7/1/11 - 6/30/14	\$440,000
Air Force Office of Scientific Research Development of the Nuclear-Electronic Orbital Approach and Applications to Water-Anion Complexes and Biomimetic Models of Hydrogenase	4/15/10 - 4/14/14	\$750,207
Department of Energy Center for Molecular Electrocatalysis (EFRC group proposal, P.I. Morris Bullock)	8/1/09 - 7/30/14	\$1,125,000 (S.H.S.)
National Institutes of Health Simulation of Proton and Hydride Transfer in Enzymes (MERIT Award)	5/1/11 - 4/30/16	\$1,421,045
Air Force Office of Scientific Research Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer Processes	9/1/14 - 3/31/18	\$644,499
National Science Foundation Non-Born-Oppenheimer Effects between Electrons and Protons	7/1/14 - 6/30/18	\$636,991
Department of Energy Center for Molecular Electrocatalysis (EFRC, P.I. Morris Bullock)	9/1/14 - 7/31/18	\$644,000 (S.H.S.)
Department of Energy Argonne-Northwestern Solar Energy Research Center (EFRC, P.I. Michael Wasielewski)	8/1/16 - 7/31/18	\$150,000 (S.H.S.)

**Current (sole P.I. Hammes-Schiffer unless otherwise noted)**

National Institutes of Health Simulation of Proton and Hydride Transfer in Enzymes (MERIT Award)	5/1/16 - 4/30/21	\$1,934,195
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Air Force Office of Scientific Research	2/15/18 – 2/14/22	\$939,683
Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer Processes in Solvated Molecules and Photoreceptor Proteins		
Air Force Office of Scientific Research	9/1/18 – 5/31/23	\$891,250 (S.H.S.)
Molecular-Scale Studies of Liquid-Solid Interfaces in Electrochemical Processes (MURI, P.I. Tim Lian)		
National Science Foundation	8/1/18 – 7/31/20	\$320,000
Non-Born-Oppenheimer Effects in the Framework of Multicomponent Time-Dependent Density Functional Theory		
Department of Energy	8/1/18 – 7/31/22	\$860,000 (S.H.S.)
Center for Molecular Electrocatalysis (CME EFRC, P.I. Morris Bullock)		
Department of Energy	8/1/18 – 7/31/22	\$400,000 (S.H.S.)
Center for Alkaline-Based Energy Solutions (CABES EFRC, P.I. Hector Abruña)		
Department of Energy	8/1/18 - 7/31/20	\$90,000 (S.H.S.)
Center for Light Energy Activated Redox Processes (LEAP EFRC, P.I. Michael Wasielewski)		
National Science Foundation	10/1/13 - 9/30/18	\$900,000 (S.H.S.)
Center for Innovation in Solar Fuels (CCI, P.I. Harry Gray)		
National Science Foundation	10/1/15 - 9/30/20	\$300,000 (S.H.S.)
Molecular Aspects of Interfaces, Fluid/Solid Mixtures, Proton and Oxygen Ion Transport in Liquids and Solids, Multiscale Methods (PIRE, P.I. Narayana Aluru)		
Department of Energy	11/1/17 – 10/31/21	\$604,000 (S.H.S.)
Advancing Catalysis Modeling: From Atomistic Chemistry to Whole System Simulation (SciDAC, P.I. Martin Head-Gordon)		
Canadian Institute for Advanced Research (CIFAR)	7/1/16 – 6/30/19	\$90,000 (S.H.S.)
Bio-inspired Solar Energy		

## 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. Nat. Acad. Sci. USA* **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. R. 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. Kobraak 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 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-methylxazole 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," *Chem. Phys.* **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).
76. C. Swalina and S. Hammes-Schiffer, "Impact of nuclear quantum effects on the molecular structure of bihalides and the hydrogen fluoride dimer," *J. Phys. Chem. A* **109**, 10410-10417 (2005).
77. E. Hatcher, A. Soudackov, and S. Hammes-Schiffer, "Comparison of dynamical aspects of nonadiabatic electron, proton, and proton-coupled electron transfer reactions," *Chem. Phys.* **319**, 93-100 (2005).

78. J. B. Watney, A. V. Soudackov, K. F. Wong, and S. Hammes-Schiffer, "Calculation of the transition state theory rate constant for a general reaction coordinate: Application to hydride transfer in an enzyme," *Chem. Phys. Lett.* **418**, 268-271 (2006).
79. S. Hammes-Schiffer, "Hydrogen tunneling and protein motion in enzyme reactions," *Acc. Chem. Res.* **39**, 93-100 (2006).
80. A. Sergi, J. B. Watney, K. F. Wong, and S. Hammes-Schiffer, "Freezing a single distal motion in dihydrofolate reductase," *J. Phys. Chem. B* **110**, 2435-2441 (2006).
81. S. Hammes-Schiffer and S. J. Benkovic, "Relating protein motion to catalysis," *Annu. Rev. Biochem.* **75**, 519-541 (2006).
82. S. J. Benkovic and S. Hammes-Schiffer, "Enzyme motions inside and out," *Science* **312**, 208-209 (2006).
83. J. B. Watney and S. Hammes-Schiffer, "Comparison of coupled motions in *Escherichia coli* and *Bacillus subtilis* dihydrofolate reductase," *J. Phys. Chem. B* **110**, 10130-10138 (2006).
84. S. Hammes-Schiffer and J. B. Watney, "Hydride transfer catalyzed by *Escherichia coli* and *Bacillus subtilis* dihydrofolate reductase: Coupled motions and distal mutations," *Phil. Trans. R. Soc. B* **361**, 1365-1373 (2006).
85. S. Y. Kim and S. Hammes-Schiffer, "Hybrid quantum/classical molecular dynamics for a proton transfer reaction coupled to a dissipative bath," *J. Chem. Phys.* **124**, 244102 (2006).
86. C. Swalina, M. V. Pak, A. Chakraborty, and S. Hammes-Schiffer, "Explicit electron-proton correlation in the nuclear-electronic orbital framework," *J. Phys. Chem. A* **110**, 9983-9987 (2006).
87. Y. A. Small, V. Guallar, A. V. Soudackov, and S. Hammes-Schiffer, "Hydrogen bonding pathways in human dihydroorotate dehydrogenase," *J. Phys. Chem. B* **110**, 19704-19710 (2006).
88. Y. Ohta, A. V. Soudackov, and S. Hammes-Schiffer, "Extended spin-boson model for nonadiabatic hydrogen tunneling in the condensed phase," *J. Chem. Phys.* **125**, 144522 (2006).
89. Q. Wang and S. Hammes-Schiffer, "Hybrid quantum/classical path integral approach for simulation of hydrogen transfer reactions in enzymes," *J. Chem. Phys.* **125**, 184102 (2006).
90. J. H. Skone, A. V. Soudackov, and S. Hammes-Schiffer, "Calculation of vibronic couplings for phenoxyl/phenol and benzyl/toluene self-exchange reactions: Implications for proton-coupled electron transfer mechanisms," *J. Am. Chem. Soc.* **128**, 16655-16663 (2006).
91. S. Hammes-Schiffer, "Proton-coupled electron transfer reactions: Theoretical formulation and applications," pp. 479-502 in *Handbook of Hydrogen Transfer. Volume 2: Physical and Chemical Aspects of Hydrogen Transfer*, eds. J. T. Hynes, J. P. Klinman, H.-H. Limbach and R. L. Schowen (Wiley-VCH, Weinheim, 2007).
92. S. J. Benkovic and S. Hammes-Schiffer, "Dihydrofolate reductase: Hydrogen tunneling and protein motion," pp. 1439-1454 in *Handbook of Hydrogen Transfer. Volume 4: Biological Aspects of Hydrogen Transfer*, eds. J. T. Hynes, J. P. Klinman, H.-H. Limbach and R. L. Schowen (Wiley-VCH, Weinheim, 2007).
93. E. Hatcher, A. V. Soudackov, and S. Hammes-Schiffer, "Proton-coupled electron transfer in soybean lipoxygenase: Dynamical behavior and temperature dependence of kinetic isotope effects," *J. Am. Chem. Soc.* **129**, 187-196 (2007).
94. M. Kumarasiri, C. Swalina, and S. Hammes-Schiffer, "Anharmonic effects in ammonium nitrate and hydroxylammonium nitrate clusters," *J. Phys. Chem. B* **111**, 4653-4658 (2007).
95. C. Swalina, Q. Wang, A. Chakraborty, and S. Hammes-Schiffer, "Analysis of nuclear quantum effects on hydrogen bonding," *J. Phys. Chem. A* **111**, 2206-2212 (2007).
96. M. V. Pak, A. Chakraborty, and S. Hammes-Schiffer, "Density functional theory treatment of electron correlation in the nuclear-electronic orbital approach," *J. Phys. Chem. A* **111**, 4522-4526 (2007).

97. H. Ishikita, A. V. Soudackov, and S. Hammes-Schiffer, "Buffer-assisted proton-coupled electron transfer in a model rhenium-tyrosine complex," *J. Am. Chem. Soc.* **129**, 11146-11152 (2007).
98. M. K. Ludlow, J. H. Skone, and S. Hammes-Schiffer, "Substituent effects on the vibronic coupling for the phenoxyl/phenol self-exchange reaction," *J. Phys. Chem. B* **112**, 336-343 (2008).
99. S. Hammes-Schiffer, E. Hatcher, H. Ishikita, J. H. Skone, and A. V. Soudackov, "Theoretical studies of proton-coupled electron transfer: Models and concepts relevant to bioenergetics," *Coord. Chem. Rev.* **252**, 384-394 (2008).
100. P. E. Adamson, X. F. Duan, L. W. Burggraf, M. V. Pak, C. Swalina, and S. Hammes-Schiffer, "Modeling positrons in molecular electronic structure calculations with the nuclear-electronic orbital method," *J. Phys. Chem. A* **112**, 1346-1351 (2008).
101. S. J. Benkovic, G. G. Hammes, and S. Hammes-Schiffer, "Free energy landscape of enzyme catalysis," *Biochemistry* **47**, 3317-3321 (2008).
102. C. Venkataraman, A. V. Soudackov, and S. Hammes-Schiffer, "Theoretical formulation of nonadiabatic electrochemical proton-coupled electron transfer at metal-solution interfaces," *J. Phys. Chem. C* **112**, 12386-12397 (2008).
103. A. Chakraborty, M. V. Pak, and S. Hammes-Schiffer, "Inclusion of explicit electron-proton correlation in the nuclear-electronic orbital approach using Gaussian-type geminal functions," *J. Chem. Phys.* **129**, 014101 (2008).  
Erratum: *J. Chem. Phys.* **134**, 079902 (2011).
104. I. Navrotskaya, A. V. Soudackov, and S. Hammes-Schiffer, "Model system-bath Hamiltonian and nonadiabatic rate constants for proton-coupled electron transfer at electrode-solution interfaces," *J. Chem. Phys.* **128**, 244712 (2008).
105. A. Chakraborty, M. V. Pak, and S. Hammes-Schiffer, "Development of electron-proton density functionals for multicomponent density functional theory," *Phys. Rev. Lett.* **101**, 153001 (2008).  
Erratum: *Phys. Rev. Lett.* **106**, 169902 (2011).
106. S. Hammes-Schiffer and A. V. Soudackov, "Proton-coupled electron transfer in solution, proteins, and electrochemistry," *J. Phys. Chem. B* **112**, 14108-14123 (2008) (Centennial Feature Article).
107. D. K. Chakravorty, M. Kumarasiri, A. V. Soudackov, and S. Hammes-Schiffer, "Implementation of umbrella integration within the framework of the empirical valence bond approach," *J. Chem. Theory and Comput.* **4**, 1974-1980 (2008).
108. A. Chakraborty and S. Hammes-Schiffer, "Density matrix formulation of the nuclear-electronic orbital approach with explicit electron-proton correlation," *J. Chem. Phys.* **129**, 204101 (2008).
109. S. Hammes-Schiffer, "Selected Theoretical Models and Computational Methods for Enzymatic Tunnelling," pp. 79-104 in *Quantum Tunnelling in Enzyme-Catalysed Reactions*, eds. R. K. Allemann and N. S. Scrutton (Royal Society of Chemistry, Cambridge, 2009).
110. S. J. Edwards, A. V. Soudackov, and S. Hammes-Schiffer, "Analysis of kinetic isotope effects for proton-coupled electron transfer reactions," *J. Phys. Chem. A* **113**, 2117-2126 (2009).
111. A. Hazra, J. H. Skone, and S. Hammes-Schiffer, "Combining the nuclear-electronic orbital approach with vibronic coupling theory: Calculation of the tunneling splitting for malonaldehyde," *J. Chem. Phys.* **130**, 054108 (2009).
112. M. V. Pak, A. Chakraborty, and S. Hammes-Schiffer, "Calculation of the positron annihilation rate in PsH with the positronic extension of the explicitly correlated nuclear-electronic orbital method," *J. Phys. Chem. A* **113**, 4004-4008 (2009).  
Correction: *J. Phys. Chem. A* (2012).
113. M. Kumarasiri, G. A. Baker, A. V. Soudackov, and S. Hammes-Schiffer, "Computational approach for ranking mutant enzymes according to catalytic reaction rates," *J. Phys. Chem. B* **113**, 3579-3583 (2009).



114. M. K. Ludlow, A. V. Soudackov, and S. Hammes-Schiffer, "Theoretical analysis of the unusual temperature dependence of the kinetic isotope effect in quinol oxidation," *J. Am. Chem. Soc.* **131**, 7094-7102 (2009).
115. I. Navrotskaya and S. Hammes-Schiffer, "Electrochemical proton-coupled electron transfer: Beyond the golden rule," *J. Chem. Phys.* **131**, 024112 (2009).
116. S. Hammes-Schiffer, "Theory of proton-coupled electron transfer in energy conversion processes," *Acc. Chem. Res.* **42**, 1881-1889 (2009).
117. L. Hammarström and S. Hammes-Schiffer, "Artificial photosynthesis and solar fuels: Guest editorial," *Acc. Chem. Res.* **42**, 1859-1860 (2009).
118. 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).
119. C. Venkataraman, A. V. Soudackov, and S. Hammes-Schiffer, "Photoinduced homogeneous proton-coupled electron transfer: Model study of isotope effects on reaction dynamics," *J. Chem. Phys.* **131**, 154502 (2009).
120. 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* **113**, 14545-14548 (2009).
121. D. K. Chakravorty, 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* **48**, 10608-10619 (2009).
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* **114**, 487-496 (2010).
123. B. Auer, M. V. Pak, and S. Hammes-Schiffer, "Nuclear-electronic orbital method within the fragment molecular orbital approach," *J. Phys. Chem. C* **114**, 5582-5588 (2010).
124. M. K. Ludlow, A. V. Soudackov, and S. Hammes-Schiffer, "Electrochemical proton-coupled electron transfer of an osmium aquo complex: Theoretical analysis of asymmetric Tafel plots and transfer coefficients," *J. Am. Chem. Soc.* **132**, 1234-1235 (2010).
125. B. Auer and S. Hammes-Schiffer, "Localized Hartree product treatment of multiple protons in the nuclear-electronic orbital framework," *J. Chem. Phys.* **132**, 084110 (2010).
126. S. J. Edwards, A. V. Soudackov, and S. Hammes-Schiffer, "Impact of distal mutation on hydrogen transfer interface and substrate conformation in soybean lipoxygenase," *J. Phys. Chem. B* **114**, 6653-6660 (2010).
127. D. K. Chakravorty and S. Hammes-Schiffer, "Impact of mutation on proton transfer reactions in ketosteroid isomerase: Insights from molecular dynamics simulations," *J. Am. Chem. Soc.* **132**, 7549-7555 (2010).
128. S. Hammes-Schiffer, "Theoretical perspectives of DNA: Editorial," *J. Phys. Chem. Lett.* **1**, 1906 (2010).
129. N. Veeraraghavan, P. C. Bevilacqua, and S. Hammes-Schiffer, "Long-distance communication in the HDV ribozyme: Insights from molecular dynamics and experiments," *J. Mol. Biol.* **402**, 278-291 (2010).
130. A. Hazra, A. V. Soudackov, and S. Hammes-Schiffer, "Role of solvent dynamics in ultrafast photoinduced proton-coupled electron transfer reactions in solution," *J. Phys. Chem. B* **114**, 12319-12332 (2010).
131. V. C. Nashine, S. Hammes-Schiffer, and S. J. Benkovic, "Coupled motions in enzyme catalysis," *Curr. Op. Chem. Biol.* **14**, 644-651 (2010).

132. S. Hammes-Schiffer and A. A. Stuchebrukhov, "Theory of coupled electron and proton transfer reactions," *Chem. Rev.* **110**, 6939-6960 (2010).
133. S. Hammes-Schiffer, "Introduction: Proton-coupled electron transfer," *Chem. Rev.* **110**, 6937-6938 (2010).
134. P. Hanoian, P. A. Sigala, D. Herschlag, and S. Hammes-Schiffer, "Hydrogen bonding in the active site of ketosteroid isomerase: Electronic inductive effects and hydrogen bond coupling," *Biochemistry* **49**, 10339-10348 (2010).
135. A. Hazra, A. V. Soudackov, and S. Hammes-Schiffer, "Isotope effects on the nonequilibrium dynamics of ultrafast photoinduced proton-coupled electron transfer reactions in solution," *J. Phys. Chem. Lett.* **2**, 36-40 (2011).
136. A. Sirjoosingh and S. Hammes-Schiffer, "Proton-coupled electron transfer versus hydrogen atom transfer: Generation of charge-localized diabatic states," *J. Phys. Chem. A* **115**, 2367- 2377 (2011).
137. N. Veeraraghavan, A. Ganguly, J.-H. Chen, P. C. Bevilacqua, S. Hammes-Schiffer, and B. L. Golden, "Metal binding motif in the active site of the HDV ribozyme binds divalent and monovalent ions," *Biochemistry* **50**, 2672-2682 (2011).
138. S. Hammes-Schiffer, "Current theoretical challenges in proton-coupled electron transfer: Electron-proton nonadiabaticity, proton relays, and ultrafast dynamics," *J. Phys. Chem. Lett.* **2**, 1410-1416 (2011).
139. B. Auer, L. E. Fernandez, and S. Hammes-Schiffer, "Theoretical analysis of proton relays in electrochemical proton-coupled electron transfer," *J. Am. Chem. Soc.* **133**, 8282-8292 (2011).
140. S. Hammes-Schiffer, "When electrons and protons get excited," *Proc. Nat. Acad. Sci. USA* **108**, 8531-8532 (2011).
141. N. Veeraraghavan, A. Ganguly, B. L. Golden, P. C. Bevilacqua, and S. Hammes-Schiffer, "Mechanistic strategies in the HDV ribozyme: Chelated and diffuse metal ion interactions and active site protonation," *J. Phys. Chem. B* **115**, 8346-8357 (2011).
142. C. Ko, M. V. Pak, C. Swalina, and S. Hammes-Schiffer, "Alternative wavefunction ansatz for including explicit electron-proton correlation in the nuclear-electronic orbital approach," *J. Chem. Phys.* **135**, 054106 (2011).
143. P. Hanoian and S. Hammes-Schiffer, "Water in the active site of ketosteroid isomerase," *Biochemistry* **50**, 6689-6700 (2011).
144. A. Sirjoosingh and S. Hammes-Schiffer, "Diabatization schemes for generating charge-localized electron-proton vibronic states in proton-coupled electron transfer systems," *J. Chem. Theory and Comput.* **7**, 2831-2841 (2011).
145. A. Sirjoosingh, M. V. Pak, and S. Hammes-Schiffer, "Derivation of an electron-proton correlation functional for multicomponent density functional theory within the nuclear-electronic orbital approach," *J. Chem. Theory and Comput.* **7**, 2689-2693 (2011).
146. B. H. Solis and S. Hammes-Schiffer, "Theoretical analysis of mechanistic pathways for hydrogen evolution catalyzed by cobaloximes," *Inorg. Chem.* **50**, 11252-11262 (2011).
147. A. V. Soudackov, A. Hazra, and S. Hammes-Schiffer, "Multidimensional treatment of stochastic solvent dynamics in photoinduced proton-coupled electron transfer processes: Sequential, concerted, and complex branching mechanisms," *J. Chem. Phys.* **135**, 144115 (2011).
148. B. H. Solis and S. Hammes-Schiffer, "Substituent effects on cobalt diglyoxime catalysts for hydrogen evolution," *J. Am. Chem. Soc.* **133**, 19036-19039 (2011).
149. G. G. Hammes, S. J. Benkovic, and S. Hammes-Schiffer, "Flexibility, diversity, and cooperativity: Pillars of enzyme catalysis," *Biochemistry* **50**, 10422-10430 (2011).

150. A. Ganguly, P. C. Bevilacqua, and S. Hammes-Schiffer, “Quantum mechanical/molecular mechanical study of the HDV Ribozyme: Impact of the catalytic metal Ion on the mechanism,” *J. Phys. Chem. Lett.* **2**, 2906-2911 (2011).
151. L. E. Fernandez, S. Horvath, and S. Hammes-Schiffer, “Theoretical analysis of the sequential proton-coupled electron transfer mechanisms for H<sub>2</sub> oxidation and production pathways catalyzed by nickel molecular electrocatalysts,” *J. Phys. Chem. C* **116**, 3171-3180 (2012).
152. S. Hammes-Schiffer, “Proton-coupled electron transfer: Classification scheme and guide to theoretical methods,” *Energy Environ. Sci.* **5**, 7696-7703 (2012).
153. S. Horvath, L. E. Fernandez, A. V. Soudackov, and S. Hammes-Schiffer, “Insights into proton-coupled electron transfer mechanisms of electrocatalytic H<sub>2</sub> oxidation and production,” *Proc. Nat. Acad. Sci. USA* **109**, 15663-15668 (2012).
154. C. Swalina, M. V. Pak, and S. Hammes-Schiffer, “Analysis of electron-positron wavefunctions in the nuclear-electronic orbital framework,” *J. Chem. Phys.* **136**, 164105 (2012).
155. A. Sirjoosingh, M. V. Pak, and S. Hammes-Schiffer, “Multicomponent density functional theory study of the interplay between electron-electron and electron-proton correlation,” *J. Chem. Phys.* **136**, 174114 (2012).
156. B. Auer, A. V. Soudackov, and S. Hammes-Schiffer, “Nonadiabatic dynamics of photoinduced proton-coupled electron transfer: Comparison of explicit and implicit solvent simulations,” *J. Phys. Chem. B* **116**, 7695- 7708 (2012).
157. B. H. Solis and S. Hammes-Schiffer, “Computational study of anomalous reduction potentials for hydrogen evolution catalyzed by cobalt dithiolene complexes,” *J. Am. Chem. Soc.* **134**, 15253-15256 (2012).
158. B. L. Golden, S. Hammes-Schiffer, P. R. Carey, P. C. Bevilacqua, “An Integrated Picture of HDV Ribozyme Catalysis,” pp. 135-167 in *Biophysics of RNA Folding*, ed. R. Russell (Springer, New York, 2013).
159. J. P. Layfield and S. Hammes-Schiffer, “Calculation of vibrational shifts of nitrile probes in the active site of ketosteroid isomerase upon ligand binding,” *J. Am. Chem. Soc.* **135**, 717-725 (2013).
160. C. Ko, B. H. Solis, A. V. Soudackov, and S. Hammes-Schiffer, “Photoinduced proton-coupled electron transfer of hydrogen-bonded *p*-nitrophenyl-phenol-methylamine complex in solution,” *J. Phys. Chem. B* **117**, 316-325 (2013).
161. S. Hammes-Schiffer, “Catalytic efficiency of enzymes: A theoretical analysis,” *Biochemistry* **52**, 2012-2020 (2013).
162. J. Chen, A. Ganguly, Z. Miswan, S. Hammes-Schiffer, P. C. Bevilacqua, and B. L. Golden, “Identification of the catalytic Mg<sup>2+</sup> ion in the hepatitis delta virus ribozyme,” *Biochemistry* **52**, 557-567 (2013).
163. L. E. Fernandez, S. Horvath, and S. Hammes-Schiffer, “Theoretical design of molecular electrocatalysts with flexible pendant amines for hydrogen production and oxidation,” *J. Phys. Chem. Lett.* **4**, 542-546 (2013).
164. S. Horvath, L. E. Fernandez, A. M. Appel, and S. Hammes-Schiffer, “pH-dependent reduction potentials and proton-coupled electron transfer mechanisms in hydrogen-producing nickel molecular electrocatalysts,” *Inorg. Chem.* **52**, 3643-3652 (2013).
165. C. T. Liu, P. Hanoian, J. B. French, T. H. Pringle, S. Hammes-Schiffer, S. J. Benkovic, “Functional significance of evolving protein sequence in dihydrofolate reductase from bacteria to humans,” *Proc. Nat. Acad. Sci. USA* **110**, 10159-10164 (2013).
166. B. H. Solis, Y. Yu, and S. Hammes-Schiffer, “Effects of ligand modification and protonation on metal oxime hydrogen evolution electrocatalysts,” *Inorg. Chem.* **52**, 6994-6999 (2013).

167. A. Sirjoosingh, M. V. Pak, C. Swalina, and S. Hammes-Schiffer, "Reduced explicitly correlated Hartree-Fock approach within the nuclear-electronic orbital framework: Theoretical formulation," *J. Chem. Phys.* **139**, 034102 (2013).
168. A. Sirjoosingh, M. V. Pak, C. Swalina, and S. Hammes-Schiffer, "Reduced explicitly correlated Hartree-Fock approach within the nuclear-electronic orbital framework: Applications to positronic molecular systems," *J. Chem. Phys.* **139**, 034103 (2013).
169. C. Ko and S. Hammes-Schiffer, "Charge-transfer excited states and proton transfer in model guanine-cytosine DNA duplexes in water," *J. Phys. Chem. Lett.* **4**, 2540-2545 (2013).
170. P. Thaplyal, A. Ganguly, B. L. Golden, S. Hammes-Schiffer, and P. C. Bevilacqua, "Thio effects and an unconventional metal ion rescue in the genomic hepatitis delta virus ribozyme," *Biochemistry* **52**, 6499-6514 (2013).
171. J. P. Layfield and S. Hammes-Schiffer, "Hydrogen tunneling in enzymes and biomimetic models," *Chem. Rev.* **114**, 3466-3494 (2014).
172. S. Chakraborty, J. Reed, M. Ross, M. J. Nilges, I. D. Petrik, S. Ghosh, S. Hammes-Schiffer, J. T. Sage, Y. Zhang, C. E. Schulz, Y. Lu, "Spectroscopic and computational study of a nonheme iron nitrosyl center in a biosynthetic model of nitric oxide reductase," *Angew. Chem. Int. Ed.* **53**, 2417-2421 (2014).
173. A. Ganguly, P. Thaplyal, E. Rosta, P. C. Bevilacqua, and S. Hammes-Schiffer, "Quantum mechanical/molecular mechanical free energy simulations of the self-cleavage reaction in the hepatitis delta virus ribozyme," *J. Am. Chem. Soc.* **136**, 1483-1496 (2014).
174. C. A. Schwerdtfeger, A. V. Soudackov, and S. Hammes-Schiffer, "Nonadiabatic dynamics of electron transfer in solution: Explicit and implicit solvent treatments that include multiple relaxation time scales," *J. Chem. Phys.* **140**, 034113 (2014).
175. J. P. Schwans, P. Hanoian, B. J. Lengerich, F. Sunden, A. Gonzalez, Y. Tsai, S. Hammes-Schiffer, and D. Herschlag, "Experimental and computational mutagenesis to investigate the positioning of a general base within an enzyme active site," *Biochemistry* **53**, 2541-2555 (2014).
176. S. Ghosh, S. Horvath, A. V. Soudackov, and S. Hammes-Schiffer, "Electrochemical solvent reorganization energies in the framework of the polarizable continuum model," *J. Chem. Theory Comput.* **10**, 2091-2102 (2014).
177. B. H. Solis and S. Hammes-Schiffer, "Proton-coupled electron transfer in molecular electrocatalysis: Theoretical methods and design principles," *Inorg. Chem.* **53**, 6427-6443 (2014).
178. S. Hu, S. C. Sharma, A. D. Scouras, A. V. Soudackov, C. A. M. Carr, S. Hammes-Schiffer, T. Alber, J. P. Klinman, "Extremely elevated room-temperature kinetic isotope effects quantify the critical role of barrier width in enzymatic C-H activation," *J. Am. Chem. Soc.* **136**, 8157-8160 (2014).
179. C. T. Liu, J. P. Layfield, R. J. Stewart III, J. B. French, P. Hanoian, J. B. Asbury, S. Hammes-Schiffer, S. J. Benkovic, "Probing the electrostatics of active site microenvironments along the catalytic cycle for *Escherichia coli* dihydrofolate reductase," *J. Am. Chem. Soc.* **136**, 10349-10360 (2014).
180. M. T. Huynh, D. Schilter, S. Hammes-Schiffer, and T. B. Rauchfuss, "Protonation of nickel-iron hydrogenase models proceeds after isomerization at nickel," *J. Am. Chem. Soc.* **136**, 12385-12395 (2014).
181. M. T. Huynh, W. Wang, T. B. Rauchfuss, and S. Hammes-Schiffer, "Computational investigation of [FeFe]-hydrogenase models: Characterization of singly and doubly protonated intermediates and mechanistic insights," *Inorg. Chem.* **53**, 10301-10311 (2014).
182. A. V. Soudackov and S. Hammes-Schiffer, "Probing nonadiabaticity in the proton-coupled electron transfer reaction catalyzed by soybean lipoxygenase," *J. Phys. Chem. Lett.* **5**, 3274-3278 (2014).
183. D. K. Bediako, B. H. Solis, D. K. Dogutan, M. M. Roubelakis, A. G. Maher, C. H. Lee, M. B.

- Chambers, S. Hammes-Schiffer, and D. G. Nocera, "Role of pendant proton relays and proton-coupled electron transfer on the hydrogen evolution reaction by nickel hangman porphyrins," *Proc. Nat. Acad. Sci. USA* **111**, 15001-15006 (2014).
184. N. M. Tubman, I. Kylänpää, S. Hammes-Schiffer, and D. M. Ceperley, "Beyond the Born-Oppenheimer approximation with quantum Monte Carlo," *Phys. Rev. A* **90**, 042507 (2014).
  185. C. T. Liu, K. Francis, J. Layfield, X. Huang, S. Hammes-Schiffer, A. Kohen, S. J. Benkovic, "Escherichia coli dihydrofolate reductase catalyzed proton and hydride transfers: Temporal order and the roles of Asp27 and Tyr100," *Proc. Nat. Acad. Sci. USA* **111**, 18231-18236 (2014).
  186. B. H. Solis, A. G. Maher, T. Honda, D. C. Powers, D. G. Nocera, and S. Hammes-Schiffer, "Theoretical analysis of cobalt hangman porphyrins: Ligand dearomatization and mechanistic implications for hydrogen evolution," *ACS Catal.* **4**, 4516-4526 (2014).
  187. S. Ghosh and S. Hammes-Schiffer, "Calculation of electrochemical reorganization energies for redox molecules at self-assembled monolayer modified electrodes," *J. Phys. Chem. Lett.* **6**, 1-5 (2015).
  188. S. Zhang, A. Ganguly, P. Goyal, J. L. Bingaman, P. C. Bevilacqua, and S. Hammes-Schiffer, "Role of the active site guanine in the glmS ribozyme self-cleavage mechanism: Quantum mechanical/molecular mechanical free energy simulations," *J. Am. Chem. Soc.* **137**, 784-798 (2015).
  189. P. Goyal, C. A. Schwerdtfeger, A. V. Soudackov, and S. Hammes-Schiffer, "Nonadiabatic dynamics of photoinduced proton-coupled electron transfer in a solvated phenol-amine complex," *J. Phys. Chem. B* **119**, 2758-2768 (2015).
  190. P. Hanoian, C. T. Liu, S. Hammes-Schiffer, and S. J. Benkovic, "Perspectives on electrostatics and conformational motions in enzyme catalysis," *Acc. Chem. Res.* **48**, 482-489 (2015).
  191. P. Thaplyal, A. Ganguly, S. Hammes-Schiffer, P. C. Bevilacqua, "Inverse thio effects in the hepatitis delta virus ribozyme reveal that the reaction pathway is controlled by metal ion charge density," *Biochemistry* **54**, 2160-2175 (2015).
  192. A. Sirjoosingh, M. V. Pak, K. R. Brorsen, and S. Hammes-Schiffer, "Quantum treatment of protons with the reduced explicitly correlated Hartree-Fock approach," *J. Chem. Phys.* **142**, 214107 (2015).
  193. K. R. Brorsen, A. Sirjoosingh, M. V. Pak, and S. Hammes-Schiffer, "Nuclear-electronic orbital reduced explicitly correlated Hartree-Fock approach: Restricted basis sets and open-shell systems," *J. Chem. Phys.* **142**, 214108 (2015).
  194. S. Hammes-Schiffer, "Proton-coupled electron transfer: Moving together and charging forward," *J. Am. Chem. Soc.* **137**, 8860-8871 (2015).
  195. P. Goyal and S. Hammes-Schiffer, "Role of solvent dynamics in photoinduced proton-coupled electron transfer in a phenol-amine complex in solution," *J. Phys. Chem. Lett.* **6**, 3515-3520 (2015).
  196. Y. Yang, I. Kylänpää, N. M. Tubman, J. T. Krogel, S. Hammes-Schiffer, and D. Ceperley. "How large are nonadiabatic effects in atomic and diatomic systems?" *J. Chem. Phys.* **143**, 124308 (2015).
  197. A. K. Harshan, T. Yu, A. V. Soudackov, and S. Hammes-Schiffer, "Dependence of vibronic coupling on molecular geometry and environment: Bridging hydrogen atom transfer and electron-proton transfer," *J. Am. Chem. Soc.* **137**, 13545-13555 (2015).
  198. M. N. Ucisik and S. Hammes-Schiffer, "Relative binding free energies of adenine and guanine to damaged and undamaged DNA in human DNA polymerase  $\eta$ : Clues for fidelity and overall efficiency," *J. Am. Chem. Soc.* **137**, 13240-13243 (2015).
  199. M. N. Ucisik and S. Hammes-Schiffer, "Comparative molecular dynamics studies of human DNA polymerase  $\eta$ ," *J. Chem. Inf. Model.* **55**, 2672-2681 (2015).
  200. A. V. Soudackov and S. Hammes-Schiffer, "Nonadiabatic rate constants for proton transfer and proton-coupled electron transfer reactions in solution: Effects of quadratic term in the vibronic coupling expansion," *J. Chem. Phys.* **143**, 194101 (2015).

201. G. M. Chambers, M. T. Huynh, Y. Li, S. Hammes-Schiffer, T. B. Rauchfuss, E. Reijerse, and W. Lubitz, "Models of the Ni-L and Ni-SI<sub>a</sub> states of the [NiFe]-hydrogenase active site," *Inorg. Chem.* **55**, 419-431 (2016).
202. B. H. Solis, A. G. Maher, D. K. Dogutan, D. G. Nocera, and S. Hammes-Schiffer, "Nickel phlorin intermediate formed by proton-coupled electron transfer in hydrogen evolution mechanism," *Proc. Nat. Acad. Sci. USA* **113**, 485-492 (2016).
203. S. Raugei, M. L. Helm, S. Hammes-Schiffer, A. M. Appel, M. O'Hagan, E. S. Wiedner, and R. M. Bullock, "Experimental and computational mechanistic studies guiding the rational design of molecular electrocatalysts for production and oxidation of hydrogen," *Inorg. Chem.* **55**, 445-460 (2016).
204. S. R. Kennedy, P. Goyal, M. N. Kozar, H. P. Yennawar, S. Hammes-Schiffer, and B. J. Lear, "Effect of protonation upon electronic coupling in the mixed valence and mixed protonated complex, [Ni(2,3-pyrazinedithiol)<sub>2</sub>]," *Inorg. Chem.* **55**, 1433-1445 (2016).
205. P. Goyal, C. A. Schwerdtfeger, A. V. Soudackov, and S. Hammes-Schiffer, "Proton quantization and vibrational relaxation in nonadiabatic dynamics of photoinduced proton-coupled electron transfer in a solvated phenol-amine complex," *J. Phys. Chem. B* **120**, 2407-2417 (2016).
206. C. W. Anson, S. Ghosh, S. Hammes-Schiffer, and S. S. Stahl, "Co(salophen)-catalyzed aerobic oxidation of para-hydroquinone: Mechanism and implications for aerobic oxidation catalysis," *J. Am. Chem. Soc.* **138**, 4186-4193 (2016).
207. A. K. Harshan, B. H. Solis, J. R. Winkler, H. B. Gray, and S. Hammes-Schiffer, "Computational study of fluorinated diglyoxime-iron complexes: Tuning the electrocatalytic pathways for hydrogen evolution," *Inorg. Chem.* **55**, 2934-2940 (2016).
208. S. Ghosh, A. V. Soudackov, and S. Hammes-Schiffer, "Electrochemical electron transfer and proton-coupled electron transfer: Effects of double layer and ionic environment on solvent reorganization energies," *J. Chem. Theory Comput.* **12**, 2917-2925 (2016).
209. D. Schilter, J. M. Camara, M. T. Huynh, S. Hammes-Schiffer, and T. B. Rauchfuss, "Hydrogenase enzymes and their synthetic models: The role of metal hydrides," *Chem. Rev.* **116**, 8693-8749 (2016).
210. M. N. Ucisik, P. C. Bevilacqua, and S. Hammes-Schiffer, "Molecular dynamics study of twister ribozyme: Role of Mg<sup>2+</sup> ions and the hydrogen-bonding network in the active site," *Biochemistry* **55**, 3834-3846 (2016).
211. O. A. Ulloa, M. T. Huynh, C. P. Richers, J. A. Bertke, M. J. Nilges, S. Hammes-Schiffer, and T. B. Rauchfuss, "Mechanism of H<sub>2</sub> production by models for the [NiFe]-hydrogenases: Role of reduced hydrides," *J. Am. Chem. Soc.* **138**, 9234-9245 (2016).
212. T. Culpitt, K. R. Brorsen, M. V. Pak, and S. Hammes-Schiffer, "Multicomponent density functional theory embedding formulation," *J. Chem. Phys.* **145**, 044106 (2016).
213. T. Yu, A. V. Soudackov, and S. Hammes-Schiffer, "Computational insights into five- versus six-coordinate iron center in ferrous soybean lipoxygenase," *J. Phys. Chem. Lett.* **7**, 3429-3433 (2016).
214. S. Zhang, D. R. Stevens, P. Goyal, J. L. Bingham, P. C. Bevilacqua, and S. Hammes-Schiffer, "Assessing the potential effects of active site Mg<sup>2+</sup> ions in the *glmS* ribozyme-cofactor complex," *J. Phys. Chem. Lett.* **7**, 3984-3988 (2016).
215. M. T. Huynh, C. W. Anson, A. C. Cavell, S. S. Stahl, and S. Hammes-Schiffer, "Quinone 1e<sup>-</sup> and 2e<sup>-</sup>/2H<sup>+</sup> reduction potentials: Identification and analysis of deviations from systematic scaling relationships," *J. Am. Chem. Soc.* **138**, 15903-15910 (2016).
216. A. V. Soudackov and S. Hammes-Schiffer, "Proton-coupled electron transfer reactions: Analytical rate constants and case study of kinetic isotope effects in lipoxygenase," *Faraday Discuss.* **195**, 171-189 (2016).

217. S. Hammes-Schiffer, “A conundrum for density functional theory,” *Science* **355**, 28-29 (2017).
218. P. Goyal and S. Hammes-Schiffer, “Tuning the ultrafast dynamics of photoinduced proton-coupled electron transfer in energy conversion processes,” *ACS Energy Lett.* **2**, 512-519 (2017).
219. M. Horitani, A. R. Offenbacher, C. A. M. Carr, T. Yu, V. Hoeke, G. E. Cutsail III, S. Hammes-Schiffer, J. P. Klinman, and B. M. Hoffman, “<sup>13</sup>C ENDOR spectroscopy of lipoxxygenase-substrate complexes reveals the structural basis for C-H activation by tunneling,” *J. Am. Chem. Soc.* **139**, 1984-1997 (2017).
220. K. R. Brorsen, M. V. Pak, and S. Hammes-Schiffer, “Calculation of positron binding energies and electron-positron annihilation rates for atomic systems with the reduced explicitly correlated Hartree-Fock method within the nuclear-electronic orbital framework,” *J. Phys. Chem. A* **121**, 515-522 (2017).
221. P. Goyal and S. Hammes-Schiffer, “Role of active site conformational changes in photocycle activation of the AppA BLUF photoreceptor,” *Proc. Nat. Acad. Sci. USA* **114**, 1480-1485 (2017).
222. J. L. Bingaman, S. Zhang, D. R. Stevens, N. H. Yennawar, S. Hammes-Schiffer, and P. C. Bevilacqua, “GlcN6P cofactor serves multiple catalytic roles in the *glmS* ribozyme,” *Nat. Chem. Biol.* **13**, 439-445 (2017).
223. M. N. Ucisik and S. Hammes-Schiffer, “Effects of active site mutations on specificity of nucleobase binding in human DNA polymerase  $\eta$ ,” *J. Phys. Chem. B* **121**, 3667-3675 (2017).
224. S. Hammes-Schiffer, “Catalysts by design: The power of theory,” *Acc. Chem. Res.* **50**, 561-566 (2017).
225. Z. K. Goldsmith, A. K. Harshan, J. B. Gerken, M. Voros, G. Galli, S. S. Stahl, and S. Hammes-Schiffer, “Characterization of NiFe oxyhydroxide electrocatalysts by integrated electronic structure calculations and spectroelectrochemistry,” *Proc. Nat. Acad. Sci. USA* **114**, 3050-3055 (2017).
226. S. Hu, A. V. Soudackov, S. Hammes-Schiffer, and J. P. Klinman, “Enhanced rigidification within a double mutant of soybean lipoxxygenase provides experimental support for vibronically nonadiabatic proton-coupled electron transfer models,” *ACS Catal.* **7**, 3569-3574 (2017).
227. K. R. Brorsen, Y. Yang, M. V. Pak, and S. Hammes-Schiffer, “Is the accuracy of density functional theory for atomization energies and densities in bonding regions correlated?” *J. Phys. Chem. Lett.* **8**, 2076-2081 (2017).
228. T. Culpitt, K. R. Brorsen, and S. Hammes-Schiffer, “Density functional theory embedding with the orthogonality constrained basis set expansion procedure,” *J. Chem. Phys.* **146**, 211101 (2017).
229. M. T. Huynh, S. J. Mora, M. Villalba, M. E. Tejada-Ferrari, P. A. Liddell, B. R. Cherry, A.-L. Teillout, C. W. Machan, C. P. Kubiak, D. Gust, T. A. Moore, S. Hammes-Schiffer, and A. L. Moore, “Concerted one-electron two-proton transfer processes in models inspired by the Tyr-His couple of photosystem II,” *ACS Cent. Sci.* **3**, 372-380 (2017). (Featured on cover.)
230. X. Yu, C.-H. Tung, W. Wang, M. T. Huynh, D. L. Gray, S. Hammes-Schiffer, and T. B. Rauchfuss, “Interplay between terminal and bridging diiron hydrides in neutral and oxidized states,” *Organometallics* **36**, 2245-2253 (2017).
231. Y. Yang, K. R. Brorsen, T. Culpitt, M. V. Pak, and S. Hammes-Schiffer, “Development of a practical multicomponent density functional for electron-proton correlation to produce accurate proton densities,” *J. Chem. Phys.* **147**, 114113 (2017).
232. K. R. Brorsen, Y. Yang, and S. Hammes-Schiffer, “Multicomponent density functional theory: Impact of nuclear quantum effects on proton affinities and geometries,” *J. Phys. Chem. Lett.* **8**, 3488-3493 (2017).
233. S. Ghosh, J. Castillo-Lora, A. V. Soudackov, J. M. Mayer, and S. Hammes-Schiffer, “Theoretical insights into proton-coupled electron transfer from a photoreduced ZnO nanocrystal to an organic radical,” *Nano Lett.* **17**, 5762-5767 (2017).
234. S. Ghosh, A. V. Soudackov, and S. Hammes-Schiffer, “Role of proton diffusion in the kinetics of

- proton-coupled electron transfer from photoreduced ZnO nanocrystals,” *ACS Nano* **11**, 10295-10302 (2017).
235. P. Li, A. V. Soudackov, and S. Hammes-Schiffer, “Fundamental insights into proton-coupled electron transfer in soybean lipoxygenase from quantum mechanical/molecular mechanical free energy simulations,” *J. Am. Chem. Soc.* **140**, 3068-3076 (2018).
236. Y. Yang, T. Culpitt, and S. Hammes-Schiffer, “Multicomponent time-dependent density functional theory: Proton and electron excitation energies,” *J. Phys. Chem. Lett.* **9**, 1765-1770 (2018).
237. D. R. Stevens and S. Hammes-Schiffer, “Exploring the role of the third active site metal ion in DNA polymerase  $\eta$  with QM/MM free energy simulations,” *J. Am. Chem. Soc.* **140**, 8965-8969 (2018).
238. K. R. Brorsen, P. Schneider, and S. Hammes-Schiffer, “Alternative forms and transferability of electron-proton correlation functionals in nuclear-electronic orbital density functional theory,” *J. Chem. Phys.* **149**, 044110 (2018).
239. Y. Yang, T. Culpitt, Z. Tao and S. Hammes-Schiffer, “Stability conditions and local minima in multicomponent Hartree-Fock and density functional theory,” *J. Chem. Phys.* **149**, 084105 (2018).
240. S. Hammes-Schiffer, “Controlling electrons and protons through theory: Molecular electrocatalysts to nanoparticles,” *Acc. Chem. Res.* **51**, 1975-1983 (2018).
241. Y.-H. Wang, Z. K. Goldsmith, P. E. Schneider, C. W. Anson, J. B. Gerken, S. Ghosh, S. Hammes-Schiffer, and S. S. Stahl, “Kinetic and mechanistic characterization of low-overpotential,  $H_2O_2$ -selective reduction of  $O_2$  catalyzed by  $N_2O_2$ -ligated cobalt complexes,” *J. Am. Chem. Soc.* **140**, 10890-10899 (2018).
242. J. J. Goings, C. R. Reinhardt, and S. Hammes-Schiffer, “Propensity for proton relay and electrostatic impact of protein reorganization in Slr1694 BLUF photoreceptor,” *J. Am. Chem. Soc.* **140**, 15241-15251 (2018).
243. E. Odella, S. J. Mora, B. L. Wadsworth, M. T. Huynh, J. J. Goings, P. A. Liddell, T. L. Groy, M. Gervaldo, L. E. Sereno, D. Gust, T. A. Moore, G. F. Moore, S. Hammes-Schiffer, and A. L. Moore, “Controlling proton-coupled electron transfer in bioinspired artificial photosynthetic relays,” *J. Am. Chem. Soc.* **140**, 15450-15460 (2018).
244. P. Li, A. V. Soudackov, and S. Hammes-Schiffer, “Impact of mutations on the binding pocket of soybean lipoxygenase: Implications for proton-coupled electron transfer,” *J. Phys. Chem. Lett.* **9**, 6444-6449 (2018).
245. E. R. Sayfutyarova, Z. K. Goldsmith, and S. Hammes-Schiffer, “Theoretical study of C-H bond cleavage via concerted proton-coupled electron transfer in fluorenyl-benzoates,” *J. Am. Chem. Soc.* (in press).
246. F. Pavošević, T. Culpitt, and S. Hammes-Schiffer, “Multicomponent coupled cluster singles and doubles theory within the nuclear-electronic orbital framework,” *J. Chem. Theory Comput.* (submitted).
247. E. R. Sayfutyarova, J. J. Goings, and S. Hammes-Schiffer, “Electron-coupled double proton transfer in the Slr1694 BLUF photoreceptor: A multireference electronic structure study,” *J. Phys. Chem. B* (submitted).
248. Z. K. Goldsmith, Y. C. Lam, A. V. Soudackov, and S. Hammes-Schiffer, “Proton discharge on a gold electrode from triethylammonium in acetonitrile: Theoretical modeling of potential-dependent kinetic isotope effects,” *J. Am. Chem. Soc.* (submitted).



Google Scholar, 11/18/18 (Hammes, SL OR Hammes-Schiffer, S)

**H-index:** 64

**Total citations:** 15,884

Web of Science, 18/18/18 (ResearcherID B-7325-2013)

**H-index:** 57

**Total citations:** 12,011

## **Textbook**

G. G. Hammes and S. Hammes-Schiffer, *Physical Chemistry for the Biological Sciences*, 2<sup>nd</sup> Edition. (John Wiley & Sons, Inc., Hoboken, 2015). ISBN: 978-1-118-85900-1

## 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 21<sup>st</sup> 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. 12<sup>th</sup> 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. 16<sup>th</sup> 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. 13<sup>th</sup> 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. 6<sup>th</sup> 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. 6<sup>th</sup> 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 Lipoxygenase: 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"
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): "Nuclear-Electronic Orbital Approach: Explicit Electron-Proton Correlation and Multicomponent Density Functional Theory"
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. American Chemical Society National Meeting, Symposium entitled Spectroscopy and Dynamics of Floppy Molecules, San Francisco, California, March 21-25, 2010 (talk): "Nuclear-Electronic Orbital Approach: Explicit Electron-Proton Correlation and Multicomponent Density Functional Theory"
193. 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"
194. University of South Carolina, Columbia, South Carolina, April 16, 2010 (H. Willard Davis lecture): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
195. Gordon Research Conference on Enzymes, Coenzymes, and Metabolic Pathways, Waterville Valley, New Hampshire, July 18-23, 2010 (invited talk): "Hydrogen Bonding, Electrostatics, and Conformational Motions in Enzyme Catalysis"
196. Gordon Research Conference on Atomic and Molecular Interactions, New London, New Hampshire, July 18-23, 2010 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion Processes"
197. American Chemical Society National Meeting, Symposium entitled Molecular Models for Solar Energy Conversion and Storage, Boston, Massachusetts, August 22-26, 2010 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
198. American Chemical Society National Meeting, Symposium entitled Frontiers of Condensed Phase Theory and Simulation: A Tribute to Bruce J. Berne, Boston, Massachusetts, August 22-26, 2010 (invited talk): "Dynamics of Photoinduced Proton-Coupled Electron Transfer Reactions"
199. American Chemical Society National Meeting, Symposium entitled Density Functional Theory, Boston, Massachusetts, August 22-26, 2010 (invited talk): "Multicomponent Density Functional Theory: Development of Electron-Proton Functionals"
200. University of Paris Diderot, Paris, France, September 24, 2010 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"

201. 61<sup>st</sup> Annual Meeting of International Society of Electrochemistry, Nice, France, September 26-October 1, 2010 (invited Key-Note Lecture): “Electrochemical Proton-Coupled Electron Transfer: Theory and Applications”
202. University of Calgary, Calgary, Canada, October 18, 2010 (invited talk): “Hydrogen Tunneling and Protein Motion in Enzyme Reactions”
203. Wayne State University Physics Department, Detroit, Michigan, November 4, 2010 (invited talk): “Nuclear-Electronic Orbital Approach: Quantum Calculations of Multicomponent Systems”
204. University of Chicago, Chicago, Illinois, January 31, 2011 (colloquium seminar): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
205. Gordon Research Conference on Inorganic Reaction Mechanisms, Galveston, Texas, March 6-11, 2011 (invited talk): “Proton-Coupled Electron Transfer in Inorganic Reactions”
206. American Chemical Society National Meeting, Symposium entitled Tunneling Pathways, Anaheim, California, March 27-31, 2011 (invited talk): “Proton-Coupled Electron Transfer: Proton Relays and Ultrafast Dynamics”
207. Physics Department, Pennsylvania State University, University Park, Pennsylvania, April 14, 2011 (colloquium seminar): “Electron-Proton Interactions in Complex Systems”
208. University of North Texas, Denton, Texas, April 29, 2011 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
209. Gordon Research Conference on Photochemistry, Easton, Massachusetts, July 10-15, 2011 (invited talk): “Ultrafast Dynamics of Photoinduced Proton-Coupled Electron Transfer Reactions in Solution”
210. Dynamics of Molecular Collisions Conference, Snowbird Resort, Utah, July 10-15, 2011 (invited talk): “Ultrafast Dynamics of Photoinduced Proton-Coupled Electron Transfer Reactions in Solution”
211. American Conference on Theoretical Chemistry, Telluride, Colorado, July 18-22, 2011 (invited talk): “Ultrafast Dynamics of Photoinduced Proton-Coupled Electron Transfer Reactions in Solution”
212. 15th International Conference on Biological Inorganic Chemistry (ICBIC 15), Vancouver, Canada, August 7-12, 2011 (keynote lecture): “Proton-Coupled Electron Transfer in Biological Inorganic Reactions”
213. American Chemical Society National Meeting, Symposium entitled Reduced Density Matrices in Quantum Chemistry, Denver, Colorado, August 28-September 1, 2011 (invited talk): “Avoiding the Born-Oppenheimer Separation between Electrons and Nuclei: Explicitly Correlated Wavefunctions and Multicomponent Density Functional Theory”
214. American Chemical Society National Meeting, Symposium entitled Materials Chemistry for Solar Energy Capture, Denver, Colorado, August 28-September 1, 2011 (invited talk): “Electrochemical Proton-Coupled Electron Transfer”
215. American Chemical Society National Meeting, Symposium entitled Computational Modeling of Photocatalysis and Photoinduced Charge Transfer Dynamics at Surfaces, Denver, Colorado, August 28-September 1, 2011 (invited talk): “Ultrafast Dynamics of Photoinduced Proton-Coupled Electron Transfer Reactions”
216. PCET 2011: From Biology to Catalysis, Paris, France, October 9-13, 2011 (invited talk): « Ultrafast Dynamics of Photoinduced Proton-Coupled Electron Transfer Reactions: Sequential, Concerted, and Complex Branching Mechanisms”
217. Conference on Current Trends in Computational Chemistry (CCTCC), Jackson, Mississippi, October 27-29, 2011 (invited talk): “Nuclear-Electronic Orbital Approach: Explicitly Correlated Wavefunctions and Multicomponent Density Functional Theory”
218. International Conference of Theoretical Chemistry, Berkeley, California, January 9-12, 2012 (invited talk): “Ultrafast Dynamics of Photoinduced Proton-Coupled Electron Transfer Reactions”

219. 24<sup>th</sup> Austin Symposium on Molecular Structure and Dynamics (ASMD), Dallas, Texas, March 3-6, 2012 (plenary lecture): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
220. Pennergy, the Penn Center for Energy Innovation, University of Pennsylvania, Philadelphia, Pennsylvania, March 19, 2012 (colloquium): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
221. American Chemical Society National Meeting, Symposium entitled Nonadiabatic Dynamics: Surface Hopping and Beyond, San Diego, California, March 25-29, 2012 (invited talk): “Nonadiabatic Dynamics of Ultrafast Photoinduced Proton-Coupled Electron Transfer Reactions in Solution”
222. American Chemical Society National Meeting, Symposium entitled Solar Energy Conversion and Utilization for Fuels and Energy Production, San Diego, California, March 25-29, 2012 (invited talk): “Molecular Electrocatalysts for Hydrogen Production: Electrochemical Proton-Coupled Electron Transfer”
223. American Chemical Society National Meeting, Symposium entitled Theory and Applications of Density Functional Theory, San Diego, California, March 25-29, 2012 (invited talk): “Multicomponent Density Functional Theory: Development of Electron-Proton Functionals”
224. University of Illinois, Urbana-Champaign, Illinois, April 5, 2012 (seminar): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
225. Arizona State University, Phoenix, Arizona, April 13, 2012 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
226. MIT and Harvard University, Boston, Massachusetts, April 19, 2012 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
227. 5<sup>th</sup> Argonne-Northwestern Solar Energy Research (ANSER) Center Symposium, Evanston, Illinois, April 26-27, 2012 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
228. Gordon Research Conference on Solar Fuels, Italy, May 13-18, 2012 (invited talk): “Proton-Coupled Electron Transfer in Molecular Catalysts for Solar Energy Conversion”
229. AFOSR Molecular Dynamics Contractor’s Meeting, Arlington, Virginia, May 22-24, 2012 (invited talk): “Ultrafast Dynamics of Photoinduced Proton-Coupled Electron Transfer Reactions”
230. Conference entitled Quantum Mechanics and Molecular Dynamics of Organic and Biological Reactivity, Los Angeles, California, June 21-23, 2012 (invited talk): “Hydrogen Bonding, Electrostatics, and Conformational Motions in Enzyme Catalysis”
231. Foundations of Molecular Modeling and Simulation (FOMMS) 2012, Mount Hood, Oregon, July 22-26, 2012 (invited talk): “Hydrogen Tunneling, Electrostatics, and Conformational Motions in Enzyme Catalysis”
232. Gordon Research Conference on Vibrational Spectroscopy, Biddeford, Maine, August 5-10, 2012 (invited talk): “Vibrational Stark Effect in Enzymes: Probing Electrostatics, Hydrogen Bonding, and Conformational Motions”
233. American Chemical Society National Meeting, Symposium entitled Bridging the Gap between Ab initio and Classical Simulations, Philadelphia, Pennsylvania, August 19-23, 2012 (invited talk converted to contributed talk): “Generation of Charge-Localized Electron-Proton Vibronic States for Proton-Coupled Electron Transfer Systems”
234. American Chemical Society National Meeting, Symposium entitled Electron and Energy Transfer Phenomena: At the Intersection of Electronic Structure Theory and Chemical Dynamics, Philadelphia, Pennsylvania, August 19-23, 2012 (invited talk): “Photoinduced Proton-Coupled Electron Transfer in Solution: Nonequilibrium Dynamics and Vibrational Relaxation”
235. American Chemical Society National Meeting, Symposium entitled Solvent Dynamics at Biomolecular Interfaces: Experiment and Theory, Philadelphia, Pennsylvania, August 19-23, 2012 (invited talk)

- converted to contributed talk): “Identification of Water Occupation Sites and Calculation of Vibrational Stark Shifts in the Active Site of Ketosteroid Isomerase”
236. CECAM workshop entitled Energy from the sun: Computational chemists and physicists take up the challenge, Sardinia, Italy, September 10-14, 2012 (plenary talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  237. Beckman Institute Theoretical and Computational Biophysics Seminar Series, University of Illinois at Urbana-Champaign, Illinois, September 24, 2012 (invited talk): “Hydrogen Tunneling, Electrostatics, and Conformational Motions in Enzyme Catalysis”
  238. Southeast Regional ACS meeting, symposium entitled Photonic Materials, Assemblies and Catalysts for Solar Fuels, Raleigh, North Carolina, November 14-15, 2012 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  239. Computational Science and Engineering Seminar Series, University of Illinois at Urbana-Champaign, Illinois, February 13, 2013 (invited talk): Proton-Coupled Electron Transfer in Energy Conversion Processes: Insights from Theory and Computation”
  240. American Chemical Society National Meeting, Symposium entitled Frontiers in RNA Folding and Catalysis: Interface of Theory and Experiment, New Orleans, Louisiana, April 7-11, 2013 (invited talk): “Mechanistic strategies in the HDV ribozyme: Metal ion interactions and active site protonation”
  241. American Chemical Society National Meeting, Symposium entitled ACS Award for Computers in Chemical & Pharmaceutical Research, New Orleans, Louisiana, April 7-11, 2013 (invited talk): “Avoiding the Born-Oppenheimer separation between electrons and protons in wavefunction and density functional theory calculations”
  242. International Conference on Chemical Bonding, Kauai, Hawaii, July 4-8, 2013 (invited talk): “Avoiding the Born-Oppenheimer separation between electrons and protons: Explicitly correlated wavefunctions and multicomponent density functional theory”
  243. Telluride workshop on Quantum Effects in Condensed Phase Systems, Telluride, Colorado, July 8-12, 2013 (invited talk): “Avoiding the Born-Oppenheimer separation between electrons and protons: Explicitly correlated wavefunctions and multicomponent density functional theory”
  244. Telluride workshop on Role of Dynamics in Enzyme Catalyzed Reactions, Telluride, Colorado, July 29-August 2, 2013 (invited talk): “Hydrogen Tunneling, Electrostatics, and Conformational Motions in Enzyme Catalysis”
  245. American Chemical Society National Meeting, Symposium entitled Electrostatics in Biological Systems, Indianapolis, Indiana, September 8-12, 2013 (invited talk): “Calculation of Vibrational Shifts of Nitrile Probes in Enzymes: Electrostatics, Hydrogen Bonding, and Reorganization”
  246. American Chemical Society National Meeting, Symposium entitled Non-Precious Metal Catalysis: Opportunities and Impacts, Indianapolis, Indiana, September 8-12, 2013 (invited talk): “Proton-Coupled Electron Transfer Mechanisms of Hydrogen-Producing Cobalt and Nickel Molecular Electrocatalysts”
  247. American Chemical Society National Meeting, Symposium entitled Computational Photocatalysis, Indianapolis, Indiana, September 8-12, 2013 (invited talk): “Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer Processes”
  248. Symposium on Catalytic Concepts for Energy, University of Illinois at Urbana-Champaign, Urbana, Illinois, September 13, 2013 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  249. Boston College, Boston, Massachusetts, October 3, 2013 (invited talk): “Hydrogen Tunneling, Electrostatics, and Conformational Motions in Enzyme Catalysis”
  250. Workshop entitled Fuels from Sunlight, Institute for Pure and Applied Mathematics (IPAM), University of California at Los Angeles, Los Angeles, California, October 14-18, 2013 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”

251. Symposium for the Institute for Computational Molecular Science, Temple University, Philadelphia, Pennsylvania, October 17-18, 2013 (invited talk): "Hydrogen Tunneling, Electrostatics, and Conformational Motions in Enzyme Catalysis"
252. Watkins Visiting Professorship, Wichita State University, Wichita, Kansas, November 4, 2013 (invited public talk): "How do Biological Enzymes Work?"
253. Watkins Visiting Professorship, Wichita State University, Wichita, Kansas, November 5, 2013 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
254. Molecular Biophysics Training Grant 26<sup>th</sup> Annual Research Symposium, Beckman Institute, Urbana, Illinois, November 8, 2013 (plenary talk): "Hydrogen Tunneling, Electrostatics, and Conformational Motions in Enzyme Catalysis"
255. Biophysical Society Meeting, Symposium entitled Applications of Quantum Mechanics to Biophysical Problems, San Francisco, California, February 15-19, 2014 (invited talk): "Hydrogen Tunneling, Electrostatics, and Conformational Motions in Enzyme Catalysis"
256. University of Southern California, Los Angeles, California, March 31, 2013 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
257. Distinguished Lecture in Theoretical and Computational Chemistry, University of California at San Diego, San Diego, California, April 1, 2014 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
258. Haines Lecture, University of South Dakota, April 7, 2014 (invited talk): "Proton-Coupled Electron Transfer in Energy Conversion Processes"
259. Colloquium, University of Rochester, April 9, 2014 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
260. CECAM workshop entitled Investigating Fine Quantum Effects in Biological Systems: Toward a Synergy between Experimental and Theoretical Approaches, Paris, France May 28-30, 2014 (invited talk): "Proton-Coupled Electron Transfer in Biological Systems"
261. Promoting Female Excellence in Theoretical and Computational Chemistry II, Oslo, Norway, June 13-15, 2014 (plenary talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
262. PCET 2014: Second International Conference on Proton-Coupled Electron Transfer, Uppsala, Sweden, June 15-19, 2014 (invited talk): "Theoretical Perspectives of Proton-Coupled Electron Transfer and Applications to Catalysis"
263. International Conference on Hydrogen Atom Transfer, Rome, Italy, June 22-26, 2014 (invited talk): "Theoretical Perspectives of Proton-Coupled Electron Transfer and Applications to Catalysis"
264. American Conference of Theoretical Chemistry, Telluride, Colorado, July 20-25, 2014 (invited talk): "Theoretical Perspectives of Proton-Coupled Electron Transfer and Applications to Catalysis"
265. American Chemical Society National Meeting, Symposium entitled Renewable Energy Generation at the Interface between Theory and Experiment, San Francisco, California, August 10-14, 2014 (invited talk): "Theoretical Design of Hydrogen-Evolving Molecular Electrocatalysts"
266. American Chemical Society National Meeting, Symposium entitled Photoinduced Proton Transfer (PPT) in Chemistry and Biology, San Francisco, California, August 10-14, 2014 (invited talk converted to contributed): "Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer Processes"
267. American Chemical Society National Meeting, Symposium entitled Modeling the Effects of Water and Solvation in Biological Systems: Developments and Applications, San Francisco, California, August 10-14, 2014 (invited talk): "Probing Electrostatics and Hydration in Active Site Microenvironments along the Catalytic Cycle of an Enzyme"
268. Northwestern University, Evanston, Illinois, October 24, 2014 (colloquium): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"



269. Princeton Center for Theoretical Science, Workshop on Numerical Approaches to Nonadiabatic Dynamics, November 21-22, 2014 (invited talk): "Avoiding the Born-Oppenheimer separation between electrons and protons: Nuclear-electronic orbital techniques and nonadiabatic dynamics"
270. NCSA Colloquium, University of Illinois at Urbana-Champaign, Urbana, Illinois, February 6, 2015 (invited talk): "Computer Simulation of Chemical and Biological Processes"
271. G. Wilse Robinson Lectureship, Texas Tech University, Lubbock, Texas, February 18, 2015 (invited departmental seminar): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
272. G. Wilse Robinson Lectureship, Texas Tech University, Lubbock, Texas, February 19, 2015 (invited public lecture): "Enzymes: The Engines of Biology"
273. Computational Molecular Science 2015, Warwick, England, March 15-18, 2015 (keynote talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
274. American Chemical Society National Meeting, Symposium entitled Modeling Excited States of Complex Systems, Denver, Colorado, March 22-26, 2015 (invited talk): "Photoinduced Proton-Coupled Electron Transfer in Solution: Quantum Mechanical/Molecular Mechanical Nonadiabatic Dynamics"
275. American Chemical Society National Meeting, Session entitled Nonadiabatic Dynamics in Symposium entitled Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular, and Condensed-Phase Systems, Denver, Colorado, March 22-26, 2015 (invited talk converted to contributed talk): "Avoiding the Born-Oppenheimer Separation between Electrons and Protons in Wavefunction and Density Functional Theory Calculations"
276. American Chemical Society National Meeting, Symposium entitled Modeling Complex Biomolecules; From Structure to Dynamics & Function, Denver, Colorado, March 22-26, 2015 (invited talk): "Proton-Coupled Electron Transfer in Soybean Lipooxygenase: Hydrogen Tunneling and Conformational Motions"
277. American Chemical Society National Meeting, Symposium entitled Molecular Catalysts for Solar Fuels, Denver, Colorado, March 22-26, 2015 (invited talk): "Theoretical Design of Hydrogen-Evolving Molecular Electrocatalysts"
278. American Chemical Society National Meeting, Symposium entitled ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of David A. Case, Denver, Colorado, March 22-26, 2015 (invited talk): "Mechanistic Strategies in the HDV Ribozyme: Metal Ion Identity Controls the Reaction Pathway"
279. Reilly Lecture, University of Notre Dame, Notre Dame, Indiana, April 13, 2015 (invited talk): "Hydrogen Tunneling, Electrostatics, and Conformational Motions in Enzyme Catalysis"
280. Reilly Lecture, University of Notre Dame, Notre Dame, Indiana, April 14, 2015 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
281. Reilly Lecture, University of Notre Dame, Notre Dame, Indiana, April 15, 2015 (invited talk): "Avoiding the Born-Oppenheimer Separation between Electrons and Protons in Molecular Orbital and Density Functional Theory"
282. International Solar Fuels Conference (ISF-1), Uppsala, Sweden, April 26-May 1, 2015 (invited talk): "Theoretical Design of Hydrogen-Evolving Molecular Electrocatalysts"
283. University of Washington, Symposium on Chemical Dynamics and the Rabinovitch Legacy, Seattle, Washington, May 30, 2015 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
284. Conference on Modeling and Simulation of Biological and Macromolecular Systems, Changchun, Jilin Province, China, June 4-7, 2015 (invited talk): "Proton-Coupled Electron Transfer: Hydrogen Tunneling and Conformational Motions"
285. International Congress of Quantum Chemistry, Beijing, China, June 8-13, 2015 (plenary talk): "Avoiding the Born-Oppenheimer Separation between Electrons and Protons:"

- Explicitly Correlated Wavefunctions and Multicomponent Density Functional Theory”
286. Telluride Workshop on Quantum Effects in Condensed Phase Systems, Telluride, Colorado, July 20-25 (invited talk): “Theoretical Perspectives of Proton-Coupled Electron Transfer”
  287. Penn Conference on Theoretical Chemistry (PCTC 2015), Philadelphia, Pennsylvania, July 29-31, 2015 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  288. American Chemical Society National Meeting, Symposium entitled Calculating  $pK_a$ 's and Redox Potentials, Boston, Massachusetts, August 16-20, 2015 (invited talk): “Calculating  $pK_a$ 's, Reduction Potentials, and Reorganization Energies for Electrochemical Proton-Coupled Electron Transfer Processes”
  289. American Chemical Society National Meeting, Symposium entitled The Role of the Outer Coordination Sphere on the Activity of Enzymes and Molecular Catalysts, Boston, Massachusetts, August 16-20, 2015 (invited talk): “Pendant Proton Relays and Ligand Non-Innocence in Hydrogen-Evolving Molecular Electrocatalysts”
  290. American Chemical Society National Meeting, Symposium for the 2015 ACS Catalysis Lectureship for the Advancement of Catalytic Science, Boston, Massachusetts, August 16-20, 2015 (invited talk): “Theoretical Design of Hydrogen-Evolving Molecular Electrocatalysts”
  291. Midwest Computational Biomolecular Modeling Symposium, Beckman Institute, University of Illinois. Urbana, Illinois, September 15-16, 2015 (invited talk): “Computational Macromolecular Modeling: Future Directions”
  292. University of Minnesota, Energy Frontier Research Center, Minneapolis, Minnesota, October 4, 2016 (invited after dinner talk): “How Centers Make a Difference”
  293. University of Minnesota, Minneapolis, Minnesota, October 5, 2016 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  294. Mathematical Biosciences Institute Workshop on Multiple Faces of Biomolecular Electrostatics, Ohio State University, Columbus, Ohio, October 12-16, 2015 (key note talk): “Probing Electrostatics and Conformational Motions in Enzyme Catalysis”
  295. Georgia Institute of Technology, Atlanta, Georgia, November 2, 2015 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  296. Emory University, Atlanta, Georgia, November 3, 2015 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  297. Yale University, Symposium for John Tully, New Haven, Connecticut, November 7, 2015 (invited talk): “Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer Processes”
  298. Pacifichem 2015, Symposium entitled Recent Progress in Molecular Theory for Excited-State Electronic Structure and Dynamics, Honolulu, Hawaii, December 15-20, 2015 (invited talk): “Photoinduced Proton-Coupled Electron Transfer in Solution: Quantum Mechanical/Molecular Mechanical Nonadiabatic Dynamics”
  299. Pacifichem 2015, Symposium entitled Molecular Catalysis of Water Splitting Reactions, Honolulu, Hawaii, December 15-20, 2015 (invited talk): “Theoretical Design of Hydrogen-Evolving Molecular Electrocatalysts”
  300. Pacifichem 2015, Symposium entitled Dynamical Intermolecular Interactions for Biological Functions, Honolulu, Hawaii, December 15-20, 2015 (invited talk): “Probing Electrostatics and Conformational Motions along the Catalytic Cycle of an Enzyme”
  301. Gordon Research Conference on Electrochemistry, Ventura, California, January 10-15, 2016 (invited talk): “Theoretical Design of Hydrogen-Evolving Molecular Electrocatalysts”
  302. University of California at Los Angeles, Los Angeles, California, January 13, 2016 (Distinguished Lecture): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  303. Jean Dreyfus Boissevain Lectureship, University of Colorado at Denver, Denver, Colorado, March 9,

- 2016 (invited named lecture): “Enzymes: The Engines of Biology”
304. Jean Dreyfus Boissevain Lectureship, University of Colorado at Denver, Denver, Colorado, March 10, 2016 (invited public lecture): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  305. University of Colorado, Boulder, Colorado, March 11, 2016 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  306. National Plenary Lecture at American Chemical Society National Meeting, San Diego, California, March 13-17, 2016 (invited National Lecture): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  307. American Chemical Society National Meeting, Symposium entitled Computational Enzymology, San Diego, California, March 13-17, 2016 (invited talk): “Probing Electrostatics and Conformational Motions along the Catalytic Cycle of Dihydrofolate Reductase”
  308. American Chemical Society National Meeting, Symposium entitled Computational Materials Chemistry, San Diego, California, March 13-17, 2016 (invited talk): “Avoiding the Born-Oppenheimer Separation between Electrons and Protons: Explicitly Correlated Wavefunctions and Multicomponent Density Functional Theory”
  309. American Chemical Society National Meeting, Symposium entitled Structure and Dynamics in Enzymatic Catalysis across Multiple Timescales: Experiment and Theory, San Diego, California, March 13-17, 2016 (invited talk): “Proton-Coupled Electron Transfer in Soybean Lipoxigenase: Hydrogen Tunneling and Conformational Motions”
  310. Walter Kauzmann Lecturer, Princeton University, Princeton, New Jersey, April 18, 2016 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  311. AFOSR Molecular Dynamics Contractor’s Meeting, Arlington, Virginia, May 24-26, 2016 (invited talk): “Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer”
  312. EMBO Conference entitled The Biochemistry and Chemistry of Biocatalysis: From Understanding to Design, Oulu, Finland, June 12-15, 2016 (invited talk): “Probing Electrostatics and Conformational Motions along the Catalytic Cycle of an Enzyme”
  313. Empirical Valence Bond Conference, Uppsala, Sweden, June 23-25, 2016 (invited talk): “Theory of Proton-Coupled Electron Transfer”
  314. 8<sup>th</sup> Molecular Quantum Mechanics Conference, Uppsala, Sweden, June 26 -July 1, 2016 (invited talk): “Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer”
  315. Gordon Research Conference on Molecular Interactions and Dynamics, Stonehill, Massachusetts, July 10-15, 2016 (invited talk): “Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer Processes”
  316. Gordon Research Conference on Computational Chemistry, Girona, Spain, July 24-28, 2016 (invited talk): “Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer”
  317. American Chemical Society National Meeting, Symposium entitled QM/MM Simulation of Chemical and Biochemical Reaction Pathways: Recent Developments and Applications, Philadelphia, Pennsylvania, August 21-25, 2016 (invited talk): “Mechanistic Strategies in Ribozymes: Catalytic Roles of Metal Ions, Nucleobases, and Cofactors”
  318. American Chemical Society National Meeting, Symposium entitled Dynamics of Natural and Artificial Systems for Energy Conversion: Insights Gained from Spectroscopic Methods and Theory, Philadelphia, Pennsylvania, August 21-25, 2016 (invited talk): “Electrochemical and Photoinduced Proton-Coupled Electron Transfer in Energy Conversion Processes”
  319. American Chemical Society National Meeting, Symposium entitled Computational Chemistry for Energy Application, Philadelphia, Pennsylvania, August 21-25, 2016 (invited talk): “Theoretical Design of Hydrogen-Evolving Molecular Electrocatalysts”
  320. Theory and Applications of Computational Chemistry, Seattle, Washington, August 28 – September 2,

- 2016 (invited plenary lecture): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
321. Institute for Sustainability, Energy, and Environment (iSEE) Congress 2016 on Energy 2030: Paths to a Sustainable Future, September 12-14, 2016 (invited talk): “Solar Energy through Better Chemistry”
  322. Faraday Discussion on Chemical Reaction Rate Theory, Cambridge, United Kingdom, September 19-21, 2016 (invited headline speaker): “Proton-Coupled Electron Transfer Reactions: Analytical Rate Constants and Case Study of Kinetic Isotope Effects in Lipoxxygenase”
  323. Thomas-Young Centre (TYC) for Materials Modelling, London, United Kingdom, September 22, 2016 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  324. University of Bristol, Bristol, United Kingdom, September 23, 2016 (invited talk): “Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer Processes”
  325. CIFAR Bio-Inspired Solar Energy Meeting, Montreal, Canada, October 28-29, 2016 (invited talk): “Inspiration from Biology: Coupling Electrons and Protons and Facilitating Tunneling”
  326. Brooklyn College, New York, New York, November 22, 2016 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  327. Northeastern University, Boston, Massachusetts, January 18, 2017 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  328. Northwestern University, Evanston, Illinois, February 2, 2017 (invited talk): “Proton-Coupled Electron Transfer in Energy Conversion Processes”
  329. Armstrong Lecture, Vanderbilt University, Nashville, Tennessee, February 24, 2017 (named lecture): “Enzyme Catalysis through the Lens of Theory”
  330. Brandeis University, Boston, Massachusetts, March 6, 2017 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  331. Greater Boston Area Theoretical Chemistry Lecture, MIT, Harvard, Boston University, Boston, Massachusetts, March 8, 2017 (invited talk): “Proton-Coupled Electron Transfer: Theory and Applications”
  332. American Chemical Society National Meeting, Symposium entitled Multicenter Molecules and Coupled Molecular Assemblies – Synthesis, Characterization, and Theory, San Francisco, California, April 2-6, 2017 (invited talk): “Theoretical Studies of Homogeneous and Heterogeneous Multicenter Electrocatalysts”
  333. American Chemical Society National Meeting, Symposium entitled Light-Driven Chemistry: Photoelectrochemistry and Photocatalysis, San Francisco, California, April 2-6, 2017 (invited talk): “Photoinduced Proton-Coupled Electron Transfer in Solvated Molecular Systems and Photoreceptor Proteins”
  334. American Chemical Society National Meeting, Symposium entitled Strong Electron Correlation and Nonadiabatic Dynamics, San Francisco, California, April 2-6, 2017 (invited talk): “Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer Processes”
  335. W. A. Noyes Distinguished Lecture, University of Texas at Austin, Austin, Texas, April 20, 2017 (named lecture): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  336. Neckers Lecture, Southern Illinois University, Carbondale, Illinois, May 5, 2017 (named lecture): “Proton-Coupled Electron Transfer: Moving Together and Charging Forward”
  337. Chemical Society of Canada, Symposium entitled Quantum Coherence and Dynamics in Biological Systems, Toronto, Canada, May 29-30, 2017 (invited talk): “Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer in Solution and Photoreceptor Proteins”
  338. International Academy of Quantum Molecular Science Annual Meeting Anniversary Celebration,

- session on Future of Quantum Molecular Science, Menton, France, June 30, 2017 (invited talk): “Methods for Integrating Electronic and Nuclear Quantum Effects”
339. 2<sup>nd</sup> International Conference on Hydrogen Atom Transfer (iCHAT), Rome, Italy, July 2-6, 2017 (invited talk): “Proton-Coupled Electron Transfer in Enzymes, Artificial Photosynthesis, and Nanoparticles”
  340. 2<sup>nd</sup> International Solar Fuels Conference (ISF-2), San Diego, California, July 6-10, 2017 (plenary lecture): “Proton-Coupled Electron Transfer in Solar Energy Conversion”
  341. Penn Conference in Theoretical Chemistry (PCTC), Philadelphia, Pennsylvania, August 17-19, 2017 (invited talk): “Interfacial Electrochemical Proton-Coupled Electron Transfer”
  342. American Chemical Society National Meeting, Washington, DC, August 20-24, 2017, symposium entitled New Paradigm for Catalyst Design: From Enzymatic Function to Functional Mimics (invited talk): “Inspiration from Biology: Coupling Electrons and Protons and Facilitating Tunneling”
  343. WATOC, Munich, Germany, August 27-September 1, 2017 (invited talk): “Multicomponent Density Functional Theory: Integrating Electronic and Nuclear Quantum Effects”
  344. ACS Publications Symposium entitled Innovation in Energy Conversion – A Physical Chemistry Perspective, Dalian, China, September 24-26, 2017 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  345. Tsinghua University, Beijing, China, September 27, 2017 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  346. Klaus Schulten Memorial Symposium, University of Illinois, Urbana, Illinois, November 7-9, 2017 (invited talk): “Proton-Coupled Electron Transfer in Enzymes and Photoreceptor Proteins”
  347. Chemistry and Mathematics in Phase Space (CHAMPS) Meeting, Bristol, United Kingdom, January 15-16, 2018 (invited talk): “Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer Processes”
  348. Gordon Research Conference on Metals in Biology, Ventura, California, January 21-26, 2018 (invited talk): “Proton-Coupled Electron Transfer and the Catalytic Role of Iron in Soybean Lipoxxygenase”
  349. Virginia Tech, Highlands in Chemistry seminar series, Blacksburg, Virginia, March 2, 2018 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  350. AFOSR Workshop on Chemical Tools for Biological Processes, Dayton, Ohio, March 13, 2018 (invited talk): “Theoretical Perspectives of Proton-Coupled Electron Transfer in Biological Systems”
  351. American Chemical Society National Meeting, New Orleans, Louisiana, March 18-22, 2018, symposium entitled Computational Catalyst Design for Energy Conversion and Storage (invited talk): “Theoretical Design of Molecular Electrocatalysts with Proton Relays for Energy Conversion Processes”
  352. American Chemical Society National Meeting, New Orleans, Louisiana, March 18-22, 2018, symposium entitled PCET Photocatalysis with Inorganic Molecules and Materials (invited talk): “Proton-Coupled Electron Transfer in Artificial Photosynthesis and Photoreduced Nanoparticles”
  353. American Chemical Society National Meeting, New Orleans, Louisiana, March 18-22, 2018, symposium entitled Insights into Structure, Function, Dynamics and Evolution of Enzymatic Mechanisms (invited talk): “Proton-Coupled Electron Transfer in Soybean Lipoxxygenase: Hydrogen Tunneling, Electrostatics, and Conformational Motions”
  354. American Chemical Society National Meeting, New Orleans, Louisiana, March 18-22, 2018, symposium entitled Awards Symposium for James Mayer (invited talk): “Interfacial Proton-Coupled Electron Transfer: Interplay between Experiment and Theory”
  355. American Chemical Society National Meeting, New Orleans, Louisiana, March 18-22, 2018, symposium entitled Awards Symposium for Thomas Rauchfuss (invited talk): “Hydrogen-Evolving

- Molecular Electrocatalysts: Interplay between Experiment and Theory”
356. American Chemical Society National Meeting, New Orleans, Louisiana, March 18-22, 2018, symposium entitled Dreyfus Awards Symposium (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  357. Nebraska Cluster for Computational Chemistry (NC3) Award Lecture, University of Nebraska-Lincoln, Lincoln, Nebraska, March 30, 2018 (invited award lecture): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  358. Conference on Predictive Catalysis: Transition-Metal Reactivity by Design, Girona, Spain, April 4-6, 2018 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  359. COST Action CM1305 Conference on Explicit Control over Spin States, Berlin, Germany, April 9-11, 2018 (invited talk): “Theoretical Design of Molecular Electrocatalysts for Energy Conversion Processes”
  360. Annual Meeting of the American Society of Biochemistry & Molecular Biology (ASBMB), San Diego, California, April 21-25, 2018 (invited talk): “Proton-Coupled Electron Transfer in Soybean Lipooxygenase: Hydrogen Tunneling and Conformational Motions”
  361. Annual Yale Science and Engineering Forum, New Haven, Connecticut, May 3, 2018 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  362. University of Pennsylvania, Philadelphia, Pennsylvania, May 9, 2017 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  363. Proton-Coupled Electron Transfer (PCET 2018), Blowing Rock, North Carolina, June 10-14, 2018 (invited talk): “Interfacial Proton-Coupled Electron Transfer: Photoreduced Nanocrystals and Metal Electrodes”
  364. Weizmann Institute, Faculty of Chemistry, Lifson Memorial Lecture, Rehovot, Israel, June 18, 2018 (invited named lecture): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  365. Photoinduced Processes in Embedded Systems (PPES 2018), Pisa, Italy, June 24-27 (invited talk): “Photoinduced Proton-Coupled Electron Transfer: Integrating Electronic and Nuclear Quantum Effects”
  366. CCI Solar Fuels Capstone Meeting, Ventura, California, July 8-12 (invited talk): “Proton-Coupled Electron Transfer: Moving Together and Charging Forward”
  367. Telluride workshop on Condensed Phase Dynamics, Telluride, Colorado, July 16-20 (invited talk): “Recent Advances in the Theory of Proton-Coupled Electron Transfer”
  368. Gordon Research Conference on Electron Donor-Acceptor Interactions, Newport, Rhode Island, August 5-10, 2018 (invited talk): “Proton-Coupled Electron Transfer: Moving Together and Charging Forward”
  369. American Chemical Society National Meeting, Boston, Massachusetts, August 19-23, 2018, symposium entitled Computational Photocatalysis: Modeling of Photophysics & Photochemistry at Interfaces (plenary talk): “Interfacial Proton-Coupled Electron Transfer: Artificial Photosynthesis and Photoreduced Nanoparticles”
  370. Brookhaven National Laboratory, Upton, New York, September 10, 2018 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  371. Pennsylvania State University, University Park, Pennsylvania, October 17, 2018 (colloquium): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
  372. Musselman Visiting Scientist and Lecturer, Gettysburg College, Gettysburg, Pennsylvania October 18, 2018 (endowed lecture series): “Enzymes: The Engines of Biology”
  373. Musselman Visiting Scientist and Lecturer, Gettysburg College, Gettysburg, Pennsylvania October 18, 2018 (endowed lecture series): “Out of the Beaker and onto the Hard Drive: The Emergence of Theoretical Chemistry”

374. Musselman Visiting Scientist and Lecturer, Gettysburg College, Gettysburg, Pennsylvania October 18, 2018 (endowed lecture series): “Solar Energy through Better Chemistry”
375. Musselman Visiting Scientist and Lecturer, Gettysburg College, Gettysburg, Pennsylvania October 18, 2018 (endowed lecture series): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
376. Connecticut Valley Quantum Chemistry Meeting, Yale University, New Haven, Connecticut, October 31, 2018 (invited talk): “Multicomponent Quantum Chemistry: Integrating Electronic and Nuclear Quantum Effects”

### ***Scheduled Talks and Seminars***

377. G. M. Kosolapoff Award, Auburn University, February 13, 2019 (award talk): “Enzymes: The Engines of Biology”
378. G. M. Kosolapoff Award, Auburn University, February 14, 2019 (colloquium): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
379. Sanibel Symposium, February 17, 2019 (plenary talk): “Multicomponent Quantum Chemistry: Integrating Electronic and Nuclear Quantum Effects”
380. Kenneth S. Pitzer Lecture, University of California at Berkeley, March 19, 2019 (named lecture)
381. 47<sup>th</sup> John Stauffer Lecture and Symposium in the Sciences, University of Southern California, Los Angeles, California, March 21, 2019 (distinguished speaker)
382. Ultrafast Photoinduced Energy and Charge Transfer: Faraday Discussion, Ventura, California, April 8-10, 2019 (headline speaker)
383. University of Arizona, Tuscon, Arizona, May 2, 2019 (invited seminar): “Multicomponent Quantum Chemistry: Integrating Electronic and Nuclear Quantum Effects”
384. 24<sup>th</sup> John Stauffer Lecturer in Chemistry, Stanford University, Stanford, California, May 14-16, 2019 (named lecturer)
385. International Society of Theoretical Chemical Physics (ISTCP), University of Tromso, Tromso, Norway, July 11-17, 2019 (opening keynote lecture)
386. Faraday Discussion meeting on Quantum Effects in Complex Systems, Warwick, Coventry, United Kingdom, September 11-13, 2019 (Closing Remarks Speaker)
387. 3<sup>rd</sup> International Conference on Hydrogen Atom Transfer (iCHAT), Rome, Italy, June 21-25, 2020 (invited talk)
388. World Association of Theoretical and Computational Chemists, Vancouver, Canada, August 16-21, 2020 (invited talk)

## 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, Fall 2010, Fall 2011

### University of Illinois

Chem 442, Introduction to Quantum Chemistry

(undergraduate quantum mechanics)

Fall 2013, Fall 2014, Fall 2015, Fall 2016, Fall 2017

Chem 550: Advanced Quantum Dynamics

Spring 2014

### Yale University

Chem 470/570, Quantum Chemistry

(graduate quantum mechanics)

Fall 2018



## 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 28<sup>th</sup> 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.scs.uiuc.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.

Participated in panels focusing on career development and/or women in science at Gordon Research Conferences and elsewhere (e.g., Atomic and Molecular Interactions, July, 2014; Electrochemistry, January, 2016)

Co-authored textbook: G. G. Hammes and S. Hammes-Schiffer, *Physical Chemistry for the Biological Sciences*, 2<sup>nd</sup> Edition. (John Wiley & Sons, Inc., Hoboken, 2015). ISBN: 978-1-118-85900-1