Curriculum Vitae
Sharon Hammes-Schiffer

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University of Illinois at Urbana-Champaign
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Date of Birth

May 27, 1966

Education

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

Professional Experience

Swanlund Professor of Chemistry University of Illinois at Urbana-Champaign	8/12 – present
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

Senior Fellow, Canadian Institute for Advanced Research (CIFAR), 2016 – present
Fellow, Biophysical Society, 2015
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

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 BBCA 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, Morgan Hammer, Aparna Harshan, Mioy Huynh, Patrick Schneider, David Stevens, Zhen Tao, Archit Vasan

Current Postdoctoral Research Assistants

Kurt Brorsen, Yan Choi, Soumya Ghosh, Puja Goyal, Pengfei Li, Yang Yang
Michael Pak (Research Assistant Professor), 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: assistant professor, CUNY York

Jonathan Skone, Ph.D., Pennsylvania State University, 2008
current position: postdoc, UC Davis

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 Veeraraghavan, 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: postdoc, University of Minnesota

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: postdoc, Humboldt University

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, Max-Planck-Institute, Muelheim

Sixue Zhang, Ph.D., University of Illinois at Urbana-Champaign, 2016
current position: postdocr, Southern Research Institute

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: research assistant professor, University of Illinois

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

<u>Past Undergraduate Research Assistants</u>

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 6/1/96 - 5/31/00 $235,700
The Incorporation of Quantum Effects in the Simulation of Proton Transfer Reaction

Petroleum Research Fund (administered by ACS) 9/1/96 - 8/31/98 $20,000
Simulation of Proton Transport along a Linear Chain of Hydrogen-Bonded Water Molecules

Air Force Office of Scientific Research 2/1/98 - 11/30/00 $322,042
Simulation of Reaction Dynamics: Nonadiabatic and Solvation Effects

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 5/1/98 - 4/30/03 $779,607
Simulation of Proton and Hydride Transfer in Enzymes

Camille Dreyfus Teacher-Scholar Award 6/1/99 - 5/31/04 $60,000

Air Force Office of Scientific Research 12/1/00 - 11/30/03 $345,000
Simulation of Reaction Dynamics for Synthesis of Energetic Materials and Resistant Coatings

National Science Foundation 6/1/00 - 5/31/04 $385,000
Theoretical and Computational Studies of Multiple Charge Transfer Reactions in the Condensed Phase

National Science Foundation 6/1/04 - 5/31/05 $140,000
Creativity Extension

Air Force Office of Scientific Research 1/1/04 - 12/31/06 $381,926
Simulation of Reactions for the Design of Energetic Materials, Resistant Coatings, and Laser Protection Devices

National Institutes of Health 1/1/04 - 12/31/06 $139,504
Simulation of Proton and Hydride Transfer in Enzymes: Supplement

National Institutes of Health 5/1/03 - 4/30/07 $921,832
Simulation of Proton and Hydride Transfer in Enzymes

DOD PET Program 8/1/06 - 7/31/07 $60,000
Porting the Nuclear-Electronic Orbital (NEO) Method to the GAMESS Code for Air Force Applications

DARPA 1/1/07 - 12/31/07 $91,710 (S.H.S.)
Evolution-Based Design of Allosteric Control Systems in Proteins (group proposal, P.I. Rama Ranganathan)

DARPA 7/11/05 - 12/14/07 $234,980 (S.H.S.)
New Technology for Inside-Out Design of Novel Enzyme Catalysts (group proposal, P.I. David Baker)

National Science Foundation 7/1/05 - 6/30/08 $415,000
Theoretical Studies of Proton-Coupled Electron Transfer Reactions

Department of Energy 10/1/05 - 9/30/08 $114,725 (S.H.S.)
Nanoscale Building Blocks for Multi-Electron Electrocatalysis: The Oxygen Reduction Reaction in Fuel Cells and Oxygen Evolution in Water Electrolysis (in collaboration with ORNL, P.I. Gilbert Brown)

Air Force Office of Scientific Research 1/1/07 - 11/30/09 $504,000
Development of the Nuclear-Electronic Orbital Approach and Applications to Ionic Liquids and Tunneling Processes

National Science Foundation 8/15/07 - 7/31/10 $183,000 (S.H.S.)
An Integrative Approach to Metalloenzyme-Catalyzed C-H Activation (group proposal with J. M. Bollinger and C. Krebs, NSF-DFG program)

National Institutes of Health 5/1/07 - 4/30/11 $1,022,039
Simulation of Proton and Hydride Transfer in Enzymes

National Institutes of Health 6/1/09 - 4/30/11 $183,309
Simulation of Proton and Hydride Transfer in Enzymes, Administrative Supplement

National Science Foundation 7/1/08 - 6/30/11 $440,000
Theoretical Studies of Proton-Coupled Electron Transfer Reactions

National Science Foundation 8/1/08 - 7/31/13 $880,930 (S.H.S.)
Powering the Planet: A Chemical Bonding Center in the Direct Conversion of Sunlight into Chemical Fuel (CCI group proposal, P.I. Harry Gray)

National Science Foundation 7/1/11 - 6/30/14 $440,000
Theoretical Studies of Proton-Coupled Electron Transfer Reactions

Air Force Office of Scientific Research 4/15/10 - 4/14/14 $750,207
Development of the Nuclear-Electronic Orbital Approach and Applications to Water-Anion Complexes and Biomimetic Models of Hydrogenase

Department of Energy 8/1/09 - 7/30/14 $1,125,000 (S.H.S.)
Center for Molecular Electrocatalysis (EFRC group proposal, P.I. Morris Bullock)

National Institutes of Health 5/1/11 - 4/30/16 $1,421,045
Simulation of Proton and Hydride Transfer in Enzymes (MERIT Award)

Current (continued on next page)

National Institutes of Health 5/1/16 - 4/30/21 $1,934,195
Simulation of Proton and Hydride Transfer in Enzymes (MERIT Award)

Air Force Office of Scientific Research 9/1/14 - 3/31/18 $644,499
Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer Processes

National Science Foundation 7/1/14 - 6/30/18 $636,991
Non-Born-Oppenheimer Effects between Electrons and Protons

Department of Energy 9/1/14 - 8/31/18 $644,000 (S.H.S.)
Center for Molecular Electrocatalysis (EFRC, P.I. Morris Bullock)

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 8/1/16 - 7/31/18 $150,000 (S.H.S.)
Argonne-Northwestern Solar Energy Research Center (EFRC, P.I. Michael Wasielewski)

Canadian Institute for Advanced Research (CIFAR) 7/1/16 – 6/30/17 $30,000 (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. Kobrak, 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).
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Citations

Google Scholar, 4/17/17 (Hammes, SL OR Hammes-Schiffer, S)
H-index: 59
Total citations: 12,810

Web of Science, 4/17/17 (Hammes, SL OR Hammes-Schiffer, S)
H-index: 53
Total citations: 10,002

Textbook

G. G. Hammes and S. Hammes-Schiffer, *Physical Chemistry for the Biological Sciences, 2nd 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, Meridan, New Hampshire, July 22-26, 2001 (invited talk): "Molecular dynamics studies of the relation between enzyme motion and activity"
51. American Chemical Society National Meeting, Symposium on First Principles Simulation of Chemical Dynamics, Chicago, Illinois, August 26-30, 2001 (talk): "Incorporating Electronic and Nuclear Quantum Effects in the Dynamical Simulation of Proton and Hydride Transfer"
52. American Chemical Society National Meeting, Symposium on Three-Dimensional Silicon-Oxygen Cages: Materials for the 21st Century, Chicago, Illinois, August 26-30, 2001 (invited talk): "Nuclear Quantum Effects in Hydrogen Transfer Reactions for the Synthesis of Polyhedral Oligomeric Silsesquioxanes"
53. American Chemical Society National Meeting, Symposium on Hybrid QM/MM Methods for Large Molecular Systems, Chicago, Illinois, August 26-30, 2001 (invited talk): "Hybrid Approach for Simulating the Dynamics of Proton and Hydride Transfer in Enzymes"
54. Temple University, Philadelphia, Pennsylvania, October 18, 2001 (departmental colloquium): "Molecular Dynamics Studies of the Relation between Enzyme Motion and Activity"
55. Symposium on Structure and Mechanism in Biological Pathways, University Park, Pennsylvania, October 20, 2001 (invited talk): "Molecular Dynamics Studies of the Relation between Enzyme Motion and Activity"
56. Pennsylvania State University, University Park, Pennsylvania, February 15, 2002 (chemical physical seminar): "Molecular Dynamics Studies of the Relation between Enzyme Motion and Activity"
57. Maria Goeppert Mayer Interdisciplinary Symposium, San Diego, California, March 2, 2002 (keynote speaker): "Molecular Dynamics Studies of the Relation between Enzyme Motion and Activity"

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

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

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

117. American Chemical Society National Meeting, Symposium on Theoretical Determination of Energy Landscapes: Methodology and Applications, Washington, D.C., August 28-September 1, 2005 (invited talk): "Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"
118. University of Houston, Houston, Texas, September 14, 2005 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
119. University of Texas at Austin, Austin, Texas, September 15, 2005 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
120. Baker Symposium, Cornell University, Ithaca New York, October 1, 2005 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
121. University of Maryland, College Park, Maryland, October 5, 2005 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
122. Royal Society Discussion Meeting on Quantum Catalysis in Enzymes – Beyond the Transition State Theory Paradigm, London, November 14-15, 2005 (invited talk) "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"

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

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

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

170. American Chemical Society National Meeting, Symposium entitled Biological and Biomimetic Interfacial Electron Transfer, Philadelphia, Pennsylvania, August 17-21, 2008 (invited talk): "Electrochemical Proton-Coupled Electron Transfer"
171. University of Akron, Akron, Ohio, November 11, 2008 (invited talk): "Proton-Coupled Electron Transfer in Solution, Proteins, and Electrochemistry"
172. Akron Section Award Address, Akron, Ohio, November 11, 2008 (award talk): "How do Biological Enzymes Work?"
173. Osaka University Forum 2008, San Francisco, California, December 8-11, 2008 (invited talk): "Proton-Coupled Electron Transfer in Energy Conversion"
174. Workshop on Chemical Dynamics: Challenges and Approaches for a Thematic Year in Mathematics and Chemistry at the Institute for Mathematics and its Applications at the University of Minnesota, Minneapolis, Minnesota, January 12-16, 2009 (invited talk): "Nuclear-Electronic Orbital Approach: Electron-Proton Correlation, Multicomponent Density Functional Theory, and Tunneling Splittings"
175. Gordon Research Conference on Protons and Membrane Reactions, Ventura, California, February 22-27, 2009 (invited talk): "Proton-Coupled Electron Transfer Reactions in Enzymes: Hydrogen Tunneling and Protein Motion"
176. Sanibel Symposium, St. Simons Island, Georgia, February 26- March 3, 2009 (invited talk): "Proton-Coupled Electron Transfer Reactions in Enzymes: Hydrogen Tunneling and Protein Motion"
177. American Chemical Society National Meeting, Symposium entitled Advances in Electronic Structure Theory and First Principles Dynamics, Salt Lake City, Utah, March 22-26, 2009 (invited talk): "Electron-Proton Correlation in the Nuclear-Electronic Orbital Approach: Explicit Correlation and Multicomponent Density Functional Theory"
178. American Chemical Society National Meeting, Symposium entitled Functional Motions in Enzyme Catalysis, Salt Lake City, Utah, March 22-26, 2009 (invited talk): "Proton-Coupled Electron Transfer in Soybean 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. 61st 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. 24th 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, Symposiun 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. 5th 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 26th 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 Lipoxygenase: 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 Lipoxygenase: 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. 8th 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, Massachussetts, 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 Lipoxygenase"
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"

Scheduled Talks and Seminars

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 in Catalysis and Energy Conversion"
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. 2nd 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. 2nd International Solar Fuels Conference (ISF-2), San Diego, California, July 6-10, 2017 (plenary lecture): "Proton-Coupled Electron Transfer in Solar Energy Conversion"
341. 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"

342. WATOC, Munich, Germany, August 27 – September 1, 2017 (invited talk)
343. 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"
344. Virginia Tech, Highlands in Chemistry seminar series, Blacksburg, Virginia, March 2, 2018 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"

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

Chem 550: Advanced Quantum Dynamics
Spring 2014

Outreach and Education

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

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

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

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

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

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

Designed and created a web site on proton-coupled electron transfer (PCET) reactions, which are central in a wide range of chemical and biological processes, including energy conversion processes. The web site is open to the public at http://webpcet.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, 2nd Edition*. (John Wiley & Sons, Inc., Hoboken, 2015). ISBN: 978-1-118-85900-1