

Curriculum Vitae Sharon Hammes-Schiffer

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Education

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

Professional Experience

Professor of Chemistry	1/24 –
Princeton University	
Sterling Professor of Chemistry	10/21 – 12/23
Yale University	
John Gamble Kirkwood Professor of Chemistry	1/18 – 10/21
Yale University	
Swanlund Professor of Chemistry	8/12 – 12/17
University of Illinois at Urbana-Champaign	
Eberly Professor in Biotechnology	8/06 – 8/12
Pennsylvania State University	
Professor of Chemistry	7/03 – 8/12
Pennsylvania State University	
Shaffer Associate Professor of Chemistry	8/00 – 7/03
Pennsylvania State University	
Clare Boothe Luce Assistant Professor of Chemistry	8/95 – 8/00
University of Notre Dame	
Postdoctoral research scientist AT&T Bell Laboratories	9/93 – 8/95
AT&T Bell Laboratories, Murray Hill, NJ	
Postdoctoral supervisor: John C. Tully	

Honors and Awards

Emerson Center Lectureship Award, Emory University, 2022
Willard Gibbs Medal Award, American Chemical Society Chicago Section, 2021
Joseph O. Hirschfelder Prize in Theoretical Chemistry, 2021
American Chemical Society Award in Theoretical Chemistry, 2021
Royal Society of Chemistry Bourke Award, 2020
G. M. Kosolapoff Award from Auburn University, 2019
Honorary Fellow, Chinese Chemical Society, 2018
Member, Connecticut Academy of Science and Engineering (CASE), 2018
Center for Advanced Study Professor, University of Illinois Urbana-Champaign, 2017
Senior Fellow, Canadian Institute for Advanced Research (CIFAR), 2016 – 2022
Fellow, Biophysical Society, 2015
Blue Waters Professor, 2014 – 2018
Member, International Academy of Quantum Molecular Science, 2014
Member, U.S. National Academy of Sciences, 2013
Fellow, American Association for the Advancement of Science, 2013
Member, American Academy of Arts and Sciences, 2012
Fellow, American Chemical Society, 2011
National Institutes of Health MERIT Award, 2011
Fellow, American Physical Society, 2010
American Chemical Society Akron Section Award, 2008
International Academy of Quantum Molecular Science Medal, 2005
Iota Sigma Pi Agnes Fay Morgan Research Award, 2005
Alexander M. Cruickshank Lecturer, Gordon Research Conferences, 2004
National Science Foundation Creativity Extension Award, 2003
Camille Dreyfus Teacher-Scholar Award, 1999
Alfred P. Sloan Research Fellowship, 1998
Ralph E. Powe Junior Faculty Enhancement Award, Oak Ridge Associated Universities, 1998
National Science Foundation CAREER Award, 1996
National Science Foundation Graduate Fellowship in Chemistry, 1988-91
AT&T Bell Laboratories GRPW (Graduate Research Program for Women) Grant, 1988 – 92
American Institute of Chemists Student Award, 1988
Merck Index Award, Princeton University, 1988
ACS Regional Scholarship Award, 1988
William Foster Memorial Prize in Chemistry, Princeton University, 1987

Named Lectureships

Arthur William Davidson Lecture, 2024
Marcus Lecture, Washington University, 2023
Distinguished Karcher-Barton Award Lecture, University of Oklahoma, 2023
Rice-Berry Lecture, University of Chicago, 2023
Löwdin Lecturer, Uppsala University, Sweden, 2022
Emerson Center Lecture, Emory University, 2022
Seymour Rothchild Memorial Lecture, University of Rochester, 2022
Condon Lecture, University of Colorado, Boulder, 2021
Borden Lecture, University of Washington, 2020
Jean Dreyfus Lectureship for Undergraduate Institutions, Georgia Southern University, 2019
Almlöf–Gropen Lecture, University of Oslo, 2019
24th John Stauffer Lecturer in Chemistry, Stanford University, 2019
47th John Stauffer Lecture, University of Southern California, 2019
Kenneth S. Pitzer Lecture in Chemistry, University of California at Berkeley, 2019
Musselman Visiting Scientist and Lecturer, Gettysburg College, 2018
Lifson Memorial Lecture, Weizmann Institute, Israel, 2018
Nebraska Cluster for Computational Chemistry (NC3) Award Lecture, 2018
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
PNAS Editorial Board, 2021 – present
Dreyfus Foundation Review Panel, 2022 – present
Blavatnik National Awards Chemistry jury member, 2018 – present (Chair in 2022, 2023, 2024)
Representative of Chemistry Section (14) for Class I Membership Committee of the National Academy of Sciences, 2015, 2017, 2023, 2024
Council of Editors, ACS Publications, 2019 – present
Ethics Committee, ACS Publications, 2019 – present
Academic Review for Schmidt Science Fellows, 2021
Judge for Discovery Prize Competition at Stony Brook University, 2021
External reviewer for Royal Swedish Academy of Sciences Göran Gustafsson Prize in Chemistry, 2021
Member of American Academy of Arts and Sciences Class I Section 3 Membership Panel, 2016 – 2017, 2021, 2022
Chair of National Academy of Sciences Award in Chemical Sciences Selection Committee, 2019
Member of National Academy of Sciences Award in Chemical Sciences Selection Committee, 2016-2017, 2020
Member of National Academy of Sciences Award for Chemistry in Service to Society Committee, 2018
Deputy Director, DOE Center for Molecular Electrocatalysis, 2018 – 2023
Alfred P. Sloan Research Fellowship Selection Committee, 2013 – 2019
Member of BESAC (Basic Energy Sciences Advisory Committee) for the Department of Energy, 2008 – 2018
Member of Scientific Advisory Board, DOE Energy Frontier Research Center: Interfacial Dynamics in Radioactive Environments and Materials (IDREAM), PNNL, 2020 – 2022
Member of Scientific Advisory Board, DOE Energy Frontier Research Center: Inorganometallic Catalyst Design Center (ICDC), University of Minnesota, 2014 – 2021
Member of Scientific Advisory Board, DOE Hub: Joint Center for Artificial Photosynthesis, 2016 – 2019
Chair of Committee of Visitors for the National Science Foundation (NSF) Division of Chemistry, 2016
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
Ad hoc member of various NIH study sections, typically once a year, 2006 – present

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
 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

Students and Postdocs Supervised

Current Graduate Students

Shiloh Andersson, Mathew Chow, Joseph Dickinson, Rowan Goudy, Phillips Hutchison, William Lake, Ben Rousseau, Logan Smith, Rachel Stein, Matthew Tremblay, Millan Welman, Jiayun Zhong, Kevin Zhu

Current Postdoctoral Research Assistants

Chiara Aieta, Kai Cui, Jonathan Fetherolf, Chris Malbon, Eno Paenurk

Past Graduate Students

John Morelli, M.S., University of Notre Dame, 1999
Hong Hu, M.S., University of Notre Dame, 2000
Karen Drukker, Ph.D., University of Amsterdam (University of Notre Dame), 1998
Hélène Decornez, Ph.D., Pennsylvania State University, 2001
Pratul Agarwal, Ph.D., Pennsylvania State University, 2002
Nedialka Iordanova, Ph.D., Pennsylvania State University, 2003
Tzvetelin Iordanov, Ph.D., Pennsylvania State University, 2003
James Watney, Ph.D., Pennsylvania State University, 2005
Soo Young Kim, Ph.D., Pennsylvania State University, 2006
Chet Swalina, Ph.D., Pennsylvania State University, 2006
Elizabeth Hatcher, Ph.D., Pennsylvania State University, 2006
Yolanda Small, Ph.D., Pennsylvania State University, 2007
Jonathan Skone, Ph.D., Pennsylvania State University, 2008
Malika Kumarasiri, Ph.D., Pennsylvania State University, 2008
Dhruva Chakravorty, Ph.D., Pennsylvania State University, 2010
Sarah Hillard Edwards, Ph.D., Pennsylvania State University, 2010
Michelle Ludlow, Ph.D., Pennsylvania State University, 2010
Narayanan Veeraraghavan, Ph.D., Pennsylvania State University, 2011
Laura Fernandez, Ph.D., Pennsylvania State University, 2013
Yinxi Yu, M.S., Pennsylvania State University, 2013
Philip Hanoian, Ph.D., Pennsylvania State University, 2014
Brian Solis, Ph.D., University of Illinois at Urbana-Champaign, 2014
Andrew Sirjoosingh, Ph.D., University of Illinois at Urbana-Champaign, 2014
Abir Ganguly, Ph.D., University of Illinois at Urbana-Champaign, 2014
Sixue Zhang, Ph.D., University of Illinois at Urbana-Champaign, 2016
Mioy Huynh, Ph.D., University of Illinois at Urbana-Champaign, 2017
Aparna Harshan, Ph.D., University of Illinois at Urbana-Champaign, 2018
Zachary Goldsmith, Ph.D., University of Illinois at Urbana-Champaign, 2019
Tanner Culpitt, Ph.D., University of Illinois at Urbana-Champaign, 2019
David Stevens, Ph.D., Yale University, 2020
Patrick Schneider, Ph.D., Yale University, 2021
Zhen Tao, Ph.D., Yale University, 2022

Clorice Reinhardt, Ph.D., Yale University, 2022
Max Secor, Ph.D., Yale University, 2023
Daniel Konstantinovsky, Ph.D., Yale University, 2023

Past Postdoctoral Research Assistants

Margaret Hurley, January 1996 – June 1997
Jian-Yun Fang, June 1996 – June 1999
Atul Bahel, January 1999 – May 2000
Alexander Soudackov, April 1998 – June 2000
Ivan Rostov, July 1999 – June 2001
Salomon Billeter, November 1999 – June 2001
Mark Kobrak, January 2000 – August 2001
Simon Webb, August 1998 – December 2001
Claudio Carra, August 2001 – June 2003
Kim Fay Wong, October 2001 – July 2004
Michael Pak, August 2003 – August 2006
Alessandro Sergi, August 2004 – March 2005
Andres Reyes, July 2003 – June 2005
Qian Wang, August 2005 – August 2006
Yasuhito Ohta, November 2004 – November 2006
Hiroshi Ishikita, November 2005 – November 2007
Irina Navrotskaya, January 2007 – February 2009
Arindam Chakraborty, March 1, 2006 – August 2009
Charulatha Venkataraman, August 2007 – October 2009
Anirban Hazra, January 2007 – June 2011
Ben Auer, September 2008 – December 2011
Chet Swalina, November 2009 – November 2012
Chaehyuk Ko, August 2010 – July 2013
Samantha Horvath, August 2010 – September 2013
Josh Layfield, August 2011 – August 2014
Christine Schwerdtfeger, May 2012 – December 2014
Melek Nihan Ucisik, August 2014 – August 2016
Tao Yu, August 2014 – August 2016
Puja Goyal, August 2013 – August 2017
Soumya Ghosh, January 2013 – June 2017
Kurt Brorsen, June 2014 – July 2018
Yang Yang, August 2016 – July 2019
Yan Choi Lam, June 2016 – July 2020
Pengfei Li, September 2016 – August 2020
Josh Goings, September 2017 – June 2020
Elvira Sayfutyarova, January 2018 – June 2021

Fabijan Pavošević, March 2018 – August 2021
Saswata Roy, March 2020 – October 2021
Robert Warburton, December 2019 – July 2022
Qi Yu, October 2019 – September 2022
Tao E. Li, August 2021 – December 2023

Past Undergraduate Research Assistants

University of Notre Dame: Susan McGovern, Michael Niemier, Charles Vardeman
Penn State University: Jeff Meadows, Greg Baker, Tyler Garner, Ben Lengerich
Yale University: Raquel Sequeira, Eva Quittman

Research Funding

Completed

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

National Science Foundation Theoretical Studies of Proton-Coupled Electron Transfer Reactions	7/1/05 - 6/30/08	\$415,000
Department of Energy Nanoscale Building Blocks for Multi-Electron Electrocatalysis: The Oxygen Reduction Reaction in Fuel Cells and Oxygen Evolution in Water Electrolysis (in collaboration with ORNL, P.I. Gilbert Brown)	10/1/05 - 9/30/08	\$114,725 (S.H.S.)
Air Force Office of Scientific Research Development of the Nuclear-Electronic Orbital Approach and Applications to Ionic Liquids and Tunneling Processes	1/1/07 - 11/30/09	\$504,000
National Science Foundation An Integrative Approach to Metalloenzyme-Catalyzed C-H Activation (group proposal with J. M. Bollinger and C. Krebs, NSF-DFG program)	8/15/07 - 7/31/10	\$183,000 (S.H.S.)
National Institutes of Health Simulation of Proton and Hydride Transfer in Enzymes	5/1/07 - 4/30/11	\$1,022,039
National Institutes of Health Simulation of Proton and Hydride Transfer in Enzymes, Administrative Supplement	6/1/09 - 4/30/11	\$183,309
National Science Foundation Theoretical Studies of Proton-Coupled Electron Transfer Reactions	7/1/08 - 6/30/11	\$440,000
National Science Foundation Powering the Planet: A Chemical Bonding Center in the Direct Conversion of Sunlight into Chemical Fuel (CCI group proposal, P.I. Harry Gray)	8/1/08 - 7/31/13	\$880,930 (S.H.S.)
National Science Foundation Theoretical Studies of Proton-Coupled Electron Transfer Reactions	7/1/11 - 6/30/14	\$440,000
Air Force Office of Scientific Research Development of the Nuclear-Electronic Orbital Approach and Applications to Water-Anion Complexes and Biomimetic Models of Hydrogenase	4/15/10 - 4/14/14	\$750,207
Department of Energy Center for Molecular Electrocatalysis (EFRC group proposal, P.I. Morris Bullock)	8/1/09 - 7/30/14	\$1,125,000 (S.H.S.)
National Institutes of Health Simulation of Proton and Hydride Transfer in Enzymes (MERIT Award)	5/1/11 - 4/30/16	\$1,421,045
Air Force Office of Scientific Research Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer Processes	9/1/14 - 3/31/18	\$644,499
National Science Foundation Non-Born-Oppenheimer Effects between Electrons and Protons	7/1/14 - 6/30/18	\$636,991
Department of Energy Center for Molecular Electrocatalysis (EFRC, P.I. Morris Bullock)	9/1/14 - 7/31/18	\$644,000 (S.H.S.)
Department of Energy	8/1/16 - 7/31/18	\$150,000 (S.H.S.)

Argonne-Northwestern Solar Energy Research Center (EFRC, P.I. Michael Wasielewski)

National Science Foundation 10/1/13 - 9/30/18 \$900,000 (S.H.S.)
Center for Innovation in Solar Fuels (CCI, P.I. Harry Gray)

National Science Foundation 10/1/15 - 9/30/20 \$300,000 (S.H.S.)
Molecular Aspects of Interfaces, Fluid/Solid Mixtures, Proton and Oxygen Ion Transport in Liquids and Solids, Multiscale Methods (PIRE, P.I. Narayana Aluru)

National Science Foundation 8/1/18 – 7/31/20 \$320,000
Non-Born-Oppenheimer Effects in the Framework of Multicomponent Time-Dependent Density Functional Theory

Department of Energy 8/1/18 - 7/31/20 \$90,000 (S.H.S.)
Center for Light Energy Activated Redox Processes (LEAP EFRC, P.I. Michael Wasielewski)

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

Department of Energy 11/1/17 – 10/31/21 \$600,000 (S.H.S.)
Advancing Catalysis Modeling: From Atomistic Chemistry to Whole System Simulation (SciDAC, P.I. Martin Head-Gordon)

Department of Energy 8/1/18 – 7/31/22 \$860,000 (S.H.S.)
Center for Molecular Electrocatalysis (CME EFRC, P.I. Morris Bullock)

Department of Energy 8/1/18 – 7/31/22 \$400,000 (S.H.S.)
Center for Alkaline-Based Energy Solutions (CABES EFRC, P.I. Hector Abruna)

Department of Energy 8/1/22 – 7/31/23 \$100,000 (S.H.S.)
Center for Molecular Electrocatalysis (CME EFRC, P.I. Morris Bullock)

Canadian Institute for Advanced Research (CIFAR) 7/1/16 – 12/31/23 \$136,475 (S.H.S.)
Bio-inspired Solar Energy

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

National Institutes of Health 1/1/21 – 12/31/25 \$2,087,084
Coupled Protons and Electrons in Biological Systems (MIRA)

Air Force Office of Scientific Research 2/15/18 – 2/14/24 \$939,683
Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer Processes in Solvated Molecules and Photoreceptor Proteins

Air Force Office of Scientific Research 9/1/18 – 7/31/24 \$1,251,250 (S.H.S.)
Molecular-Scale Studies of Liquid-Solid Interfaces in Electrochemical Processes (MURI, P.I. Tim Lian)

National Science Foundation 8/1/20 – 7/31/24 \$680,000
Non-Born-Oppenheimer Effects in the Framework of Multicomponent Time-Dependent Density Functional Theory

Department of Energy	8/1/22 – 7/31/26	\$492,800 (S.H.S.)
Center for Alkaline-Based Energy Solutions (CABES EFRC, P.I. Hector Abruna)		
Department of Energy	9/15/20 – 9/14/25	\$1,155,973 (S.H.S.)
Center for Hybrid Approaches in Solar Energy to Liquid Fuels (CHASE Solar Hub, P.I. Gerald Meyer)		
National Science Foundation	8/1/22 – 7/31/27	\$650,000 (S.H.-S.)
Collaborative Proposal: Frameworks: Sustainable Open-Source Quantum Dynamics and Spectroscopy Software (CSSI, P.I. Xiaosong Li)		
Department of Energy	9/1/22 – 8/30/25	\$1,575,000 (total)
		\$825,000 (S.H.-S.)
Multiscale Nuclear-Electronic Orbital Quantum Dynamics in Complex Environments (CCS, P.I. Hammes-Schiffer)		

Publications

Google Scholar H-index: 84 Total citations: 27,456 (January 29, 2024)

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).
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 370. J. Zhong, A. V. Soudackov, and S. Hammes-Schiffer, “Probing nonadiabaticity of proton-coupled electron transfer in ribonucleotide reductase,” *J. Phys. Chem. Lett.* **15**, 1686-1693 (2024).
 371. A. Nilsen-Moe, C. R. Reinhardt, P. Huang, H. Agarwala, R. Lopes, M. Lasagna, S. Glover, S. Hammes-Schiffer, C. Tommos, and L. Hammarström, “Switching the proton-coupled electron transfer mechanism for non-canonical tyrosine residues in a *de novo* protein,” *Chem. Sci.* 2024, Advance Article. DOI: 10.1039/d3sc05450k
 372. J. L. Alvarez-Hernandez, X. Zhang, K. Cui, A. P. Deziel, S. Hammes-Schiffer, N. Hazari, N. Piekut, and M. Zhong, “Long-range electrostatic effects from intramolecular Lewis acid binding influence the redox properties of cobalt-porphyrin complexes,” *Chem. Sci.* (submitted).
 373. N. E. Gentry, A. Kurimoto, K. Cui, J. L. Cleron, C. M. Xiang, S. Hammes-Schiffer, and J. M. Mayer, “Hydrogen on colloidal gold nanoparticles,” *J. Am. Chem. Soc.* (submitted).
 374. R. E. Warburton, A. V. Soudackov, and S. Hammes-Schiffer, “Interfacial proton-coupled electron transfer via localized trap states on metal oxide surfaces,” *J. Phys. Chem. C* (submitted).
 375. S. Hammes-Schiffer, N. Makri, and M. Rossi, “Simulating nuclear dynamics with quantum effects,” arXiv:2302.01408

Invited Talks and Seminars

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

19. CECAM workshop on Computational Methods for Studying the Dynamics of Quantum Systems, Lyon, France, September 28-October 1, 1998 (invited talk): "Mixed Quantum/Classical Molecular Dynamics with Multiple Vibrational Quantum Modes and Mixed Electronic/Vibrational States"
20. Iowa State University (departmental seminar), Ames, Iowa, November 5, 1998: "Simulation of Multiple Proton Transfer and Proton-Coupled Electron Transfer Reactions"
21. University of Southern Illinois (departmental seminar), Carbondale, Illinois, December 4, 1998: "Simulation of Multiple Proton Transfer and Proton-Coupled Electron Transfer Reactions"
22. Sanibel Symposium, St. Augustine, Florida, February 27-March 5, 1999 (invited talk): "Multiple Proton Transfer and Proton-Coupled Electron Transfer Reactions"
23. Henry Eyring Workshop on Time-Dependent Quantum Molecular Dynamics, Brian Head, Utah, March 13-17, 1999 (invited talk): "Multistate Continuum Theory and Nonadiabatic Dynamics for Multiple Charge Transfer Reactions"
24. AFOSR HEDM Contractor's Conference, Cocoa Beach, Florida, June 8-11, 1999 (invited talk): "Nonadiabatic Dynamics of Photoexcited Reactions and Solvation Effects for Fundamental Organic Reactions"
25. American Conference on Theoretical Chemistry, Boulder, Colorado, June 27-July 2, 1999 (invited talk): "Multiple Charge Transfer Reactions in the Condensed Phase"
26. Emory University (seminar), Atlanta, Georgia, July 15, 1999: "Multiple Charge Transfer Reactions: Physical Chemistry in Biological Systems"
27. Conference on the Dynamics of Molecular Collisions, Split Rock, Pennsylvania, July 18-23, 1999 (invited talk): "Nonadiabatic Dynamics of Charge Transfer Reactions"
28. American Chemical Society National Meeting, Symposium on Nonadiabatic Processes, New Orleans, Louisiana, August 23-27, 1999 (talk): "Proton-Coupled Electron Transfer Reactions in Solution"
29. American Chemical Society National Meeting, Symposium on QM/MM Methods, New Orleans, Louisiana, August 23-27, 1999 (invited talk): "Nonadiabatic Molecular Dynamics of Charge Transfer Reactions"
30. University of Notre Dame (physical chemistry seminar), Notre Dame, Indiana, September 2, 1999 (invited talk): "Multiple Charge Transfer Reactions: Physical Chemistry in Biological Systems"
31. Cornell University, Ithaca, New York, September 16, 1999 (departmental colloquium): "Multiple Charge Transfer Reactions: Physical Chemistry in Biological Systems"
32. Syracuse University, Syracuse, New York, September 17, 1999 (departmental colloquium): "Multiple Charge Transfer Reactions: Physical Chemistry in Biological Systems"
33. Colorado State University, Fort Collins, Colorado, October 7, 1999 (physical chemistry seminar): "Multiple Charge Transfer Reactions: Physical Chemistry in Biological Systems"
34. University of Colorado, Boulder, Colorado, October 8, 1999 (physical chemistry seminar): "Multiple Charge Transfer Reactions: Physical Chemistry in Biological Systems"
35. Penn State University, University Park, Pennsylvania, October 21, 1999 (departmental colloquium): "Multiple Charge Transfer Reactions: Physical Chemistry in Biological Systems"
36. University of Illinois, Urbana, Illinois, October 27, 1999 (physical chemistry seminar): "Multiple Charge Transfer Reactions: Physical Chemistry in Biological Systems"
37. Gordon Research Conference on Metals in Biology, Ventura, California, January 23-27, 2000 (invited talk): "Theoretical Perspectives on Proton-Coupled Electron Transfer"
38. University of California, Davis, California, January 27, 2000 (physical chemistry seminar): "Multiple Charge Transfer Reactions: Physical Chemistry in Biological Systems"

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

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

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

92. University of Minnesota, Minneapolis, Minnesota, April 23, 2004 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
93. Johns Hopkins University, Baltimore, Maryland, May 4, 2004 (Ephraim and Wilma Shaw Roseman Lecturer): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
94. Canadian Society for Chemistry Conference, London, Ontario, May 29-June 1, 2004 (invited talk): "Hybrid Quantum-Classical Molecular Dynamics of Hydrogen Transfer Reactions in Enzymes"
95. Workshop on Condensed Phase Dynamics, Telluride, Colorado, July 19-23, 2004 (invited talk): "Proton-Coupled Electron Transfer"
96. MERCURY Undergraduate Research Conference, Hamilton College, July 29-31, 2004 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
97. Protein Society Annual Symposium, San Diego, California, August 15, 2004 (invited talk): "Utilization of Computational Approaches to Elucidate Enzyme Mechanisms"
98. Yale University, New Haven, Connecticut, September 14, 2004 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
99. Colorado State University, Fort Collins, Colorado, October 14, 2004 (physical chemistry seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
100. University of Colorado, Boulder, Colorado, October 15, 2004 (physical chemistry seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
101. University of Massachusetts at Amherst, Amherst, Massachusetts, November 16, 2004 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
102. Mount Holyoke College, November 17, 2004, Lucy Pickett Lecturer: "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
103. McGill University, Montreal, Canada, November 23, 2004, Donald Lecturer: "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
104. Harvard University and Massachusetts Institute of Technology, Boston, Massachusetts, December 9, 2004 (Woodward Lecture Series, Harvard/MIT physical chemistry seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
105. 19th Enzyme Mechanisms Conference, Pacific Grove, California, January 5-9, 2005 (invited talk): "Impact of Enzyme Motion on Activity"
106. Gordon Research Conference on Molecular Energy Transfer, Buellton, California, January 9-15, 2005 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
107. American Chemical Society National Meeting, Symposium on Hydrogen Bonds: Developments in Experiment and Theory, San Diego, California, March 13-17, 2005 (invited talk): "Impact of Nuclear Quantum Effects on Hydrogen Bonding and Proton Transfer Reactions"
108. Princeton University, Princeton, New Jersey, March 31, 2005 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
109. Duke University, Durham, North Carolina, April 5, 2005 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
110. University of Toronto, Chemical Biophysics Symposium, April 8-10, 2005 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
111. University of Michigan, Ann Arbor, Michigan, April 21, 2005 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
112. Texas A&M University, College Station, Texas, May 5, 2005 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
113. Mathematical Biosciences Institute, Workshop on Enzyme Dynamics, Ohio State University, May 19-21, 2005 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"

114. AFOSR Contractor's Meeting, Monterey, California, May 22-25, 2005 (invited talk): "Impact of Nuclear Quantum Effects on Hydrogen Bonding and Proton Transfer Reactions"
115. American Conference on Theoretical Chemistry, Los Angeles, California, July 16-21, 2005 (invited talk): "Proton-Coupled Electron Transfer: Analysis of Dynamics and Calculations of Couplings"
116. American Chemical Society National Meeting, Symposium on Electron Transfer Processes: Making Connections, Washington, D.C., August 28-September 1, 2005 (invited talk): "Proton-Coupled Electron Transfer Reactions in Solution and Proteins"
117. American Chemical Society National Meeting, Symposium on Theoretical Determination of Energy Landscapes: Methodology and Applications, Washington, D.C., August 28-September 1, 2005 (invited talk): "Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"
118. University of Houston, Houston, Texas, September 14, 2005 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
119. University of Texas at Austin, Austin, Texas, September 15, 2005 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
120. Baker Symposium, Cornell University, Ithaca New York, October 1, 2005 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
121. University of Maryland, College Park, Maryland, October 5, 2005 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
122. Royal Society Discussion Meeting on Quantum Catalysis in Enzymes – Beyond the Transition State Theory Paradigm, London, November 14-15, 2005 (invited talk) "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
November 16, 2005: Chair the Novartis Foundation Royal Society Discussion Meeting on "Computational Approaches to H-Transfer"
123. Pacifichem Conference, Symposium on Nonadiabatic Phenomena and Related Dynamics: Theory and Experiment, Honolulu, Hawaii, December 15-20, 2005 (invited talk): "Nonadiabatic Proton-Coupled Electron Transfer Reactions in Solution and Proteins"
124. Pacifichem Conference, Symposium on Proton Transfer/Transport: H-bonded Solids, Liquids, Clusters, and Interfaces, Honolulu, Hawaii, December 15-20, 2005 (invited talk): "Hybrid Quantum-Classical Molecular Dynamics of Hydrogen Transfer Reactions in Enzymes"
125. Gordon Research Conference on Metals in Biology, Ventura, California, January 29-February 2, 2006 (invited talk): "Proton-Coupled Electron Transfer Reactions in Solution and Proteins"
126. Biophysical Society Annual Meeting, Salt Lake City, Utah, February 18-22, 2006 (invited talk): "Impact of Enzyme Motion on Activity"
127. American Chemical Society National Meeting, Symposium on Quantum Molecular Dynamics in the Condensed Phase: Towards Bridging the Gap between Theory and Experiment, Atlanta, Georgia, March 26-30, 2006 (invited talk): "Proton-Coupled Electron Transfer and Hydrogen Atom Transfer in the Condensed Phase"
128. Argonne National Laboratory, Argonne, Illinois, April 10, 2006 (seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
129. University of Texas Southwestern Medical Center, Dallas, Texas, April 13, 2006 (seminar): "Impact of Enzyme Motion on Activity"
130. DARPA Protein Design Processes Program Review, Islamorada, Florida, April 18-20, 2006 (invited talk): "Ranking Protein Designs According to Chemical Reaction Barriers"
131. New York University, New York, New York, April 28, 2006 (colloquium): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"

132. Oak Ridge National Laboratory, Oak Ridge, Tennessee, May 10, 2006 (seminar): "Proton-Coupled Electron Transfer Reactions in Solution and Proteins"
133. 12th International Congress of Quantum Chemistry (ICQC), Kyoto, Japan, May 21-26, 2006 (invited talk): "Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"
134. ICQC satellite meeting on Reactions in Solution and Biological Systems: Potential Energy Surface and Dynamics, Kyoto, Japan, May 27-29, 2006 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
135. Gordon Research Conference on Vibrational Spectroscopy: Probing Structure and Dynamics, Biddeford, Maine, July 2-7, 2006 (invited talk): "Proton-Coupled Electron Transfer Reactions in Solution and Proteins"
136. Gordon Research Conference on Atomic and Molecular Interactions, New London, New Hampshire, July 9-14, 2006 (invited talk): "Nuclear-Electronic Orbital Approach: Calculation of Structures, Frequencies, and Couplings"
137. Telluride Workshop on Condensed Phase Dynamics, Telluride, Colorado, July 17-23, 2006 (invited talk): "Nuclear-Electronic Orbital Approach: Calculation of Structures, Frequencies, and Couplings"
138. American Chemical Society National Meeting, Symposium entitled Beyond Michael Dewar's Legacy: Modern Semiempirical MO Theory, San Francisco, California, September 10-14, 2006 (invited talk): "Impact of Enzyme Motion on Activity"
139. American Chemical Society National Meeting, Symposium entitled Fifty Years of Electron Transfer and RRKM Theories, San Francisco, California, September 10-14, 2006 (invited talk): "Proton-Coupled Electron Transfer: Couplings, Rates, and Isotope Effects"
140. Michigan State University, East Lansing, Michigan, October 6, 2006 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
141. California Institute of Technology, Pasadena, California, November 28, 2006 (invited seminar): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
142. Berkeley Mini Stat Mech Meeting, Berkeley, California, January 12-14, 2007 (invited talk): "Proton-Coupled Electron Transfer Reactions: Dynamics and Kinetic Isotope Effects"
143. Gordon Research Conference on Electrochemistry, Ventura, California, January 14-19, 2007 (invited talk): "Proton-Coupled Electron Transfer Reactions in Solution and Proteins"
144. DARPA Control of Protein Conformations Kickoff Meeting, San Francisco, California, February 1-2, 2007 (invited talk): "Elucidation of Allosteric Mechanisms with Molecular Dynamics"
145. Gordon Research Conference on Gaseous Ions: Structures, Energetics and Reactions, Ventura, California, February 25-March 2, 2007 (invited talk): "Nuclear-Electronic Orbital Approach: Calculation of Structures, Frequencies, and Couplings"
146. American Chemical Society National Meeting, Symposium entitled Measures of Accuracy and Reliability in Molecular Simulation, Chicago, Illinois, March 25-29, 2007 (invited talk): "Hybrid Quantum-Classical Molecular Dynamics of Hydrogen Transfer Reactions in Enzymes"
147. Annual Meeting of the American Society for Biochemistry and Molecular Biology, Symposium entitled Computational Studies of Mechanistic and Dynamical Aspects of Enzyme Reactions, Washington, DC, April 28-May 2, 2007 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
148. 7th Annual Symposium of the Centre for Research in Molecular Modeling (CERMM), Montreal, Canada, May 4-6, 2007 (plenary lecture): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
149. AFOSR Contractor's Conference, Irvine, California, May 20-22, 2007 (invited talk): "Nuclear-Electronic Orbital Approach: Recent Advances and Applications"

150. Molecular Quantum Mechanics International Conference, Budapest, Hungary, May 29-June 3, 2007 (invited talk): "Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"
151. Gordon Research Conference on Molecular and Cellular Bioenergetics, Andover, New Hampshire, June 17-22, 2007 (invited talk): "Proton-Coupled Electron Transfer in Proteins: Dynamics and Kinetic Isotope Effects"
152. Midwest Theoretical Chemistry Conference, Bloomington, Indiana, June 28-30, 2007 (plenary talk): "Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"
153. CECAM workshop on Theoretical and Experimental Exploration of Quantum Dynamics in Condensed Phase Chemical Systems, Dublin, Ireland, August 7-10, 2007 (invited talk): "Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"
154. American Chemical Society National Meeting, Symposium entitled Hydration: From Clusters to Solution, Boston, Massachusetts, August 19-23, 2007 (invited talk): "Role of Water in Proton-Coupled Electron Transfer Reactions"
155. American Chemical Society National Meeting, Symposium entitled Strategies in Enzymatic Oxidation Catalysis, Boston, Massachusetts, August 19-23, 2007 (invited talk): "Proton-Coupled Electron Transfer in Soybean Lipoxygenase: Dynamical Behavior and Kinetic Isotope Effects"
156. Pittsburgh University, Pittsburgh, Pennsylvania, September 20, 2007 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
157. XIV International Workshop on Quantum Atomic and Molecular Tunneling in Solids and other Condensed Phases, Houston, Texas, October 28-November 1, 2007 (invited talk): "Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"
158. 16th Conference on Current Trends in Computational Chemistry, Jackson, Mississippi, November 2-3, 2007 (invited talk): "Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"
159. Gordon Research Conference in Biomolecular Interactions and Methods, Ventura, California, January 13-18, 2008 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
160. Wayne State University, Detroit, Michigan, March 18, 2008 (invited talk, medical school): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
161. Wayne State University, Detroit, Michigan, March 19, 2008 (invited talk, physical chemistry seminar): "Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"
162. University of California Berkeley Structural and Quantitative Biology seminar, April 21, 2008 (invited talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
163. Conference on Protein Dynamics and Catalysis, Tarrytown, New York, May 2-4, 2008 (invited talk): "Proton-Coupled Electron Transfer in Soybean Lipoxygenase: Dynamical Behavior and Kinetic Isotope Effects"
164. Central East Regional ACS Meeting, Symposium entitled Theoretical Models of Solvation: Methods and Applications, Columbus, Ohio, June 11-14, 2008 (invited talk): "Proton-Coupled Electron Transfer Reactions in Solution and at Electrochemical Interfaces"
165. 13th International Workshop on Quantum Systems in Chemistry and Physics (QSCP-XIII), Lansing, Michigan, July 6-12, 2008 (invited talk): "Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations"

166. 6th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VI), Vancouver, Canada, July 19-24, 2008 (plenary talk): "Hydrogen Tunneling and Protein Motion in Enzyme Reactions"
167. 6th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VI), Vancouver, Canada, July 19-24, 2008 (invited talk): "Hybrid Quantum/Classical Molecular Dynamics of Hydrogen Transfer Reactions in Enzymes"
168. Gordon Research Conference on Electron Donor Acceptor Interactions, Newport, Rhode Island, August 3-8, 2008 (invited talk): "Proton-Coupled Electron Transfer Reactions in Solution, Proteins, and Electrochemistry"
169. American Chemical Society National Meeting, Symposium entitled Water Mediated Interactions, Philadelphia, Pennsylvania, August 17-21, 2008 (talk): "Role of Water in Proton-Coupled Electron Transfer"
170. American Chemical Society National Meeting, Symposium entitled Biological and Biomimetic Interfacial Electron Transfer, Philadelphia, Pennsylvania, August 17-21, 2008 (invited talk): "Electrochemical Proton-Coupled Electron Transfer"
171. University of Akron, Akron, Ohio, November 11, 2008 (invited talk): "Proton-Coupled Electron Transfer in Solution, Proteins, and Electrochemistry"
172. Akron Section Award Address, Akron, Ohio, November 11, 2008 (award talk): "How do Biological Enzymes Work?"
173. Osaka University Forum 2008, San Francisco, California, December 8-11, 2008 (invited talk): "Proton-Coupled Electron Transfer in Energy Conversion"
174. Workshop on Chemical Dynamics: Challenges and Approaches for a Thematic Year in Mathematics and Chemistry at the Institute for Mathematics and its Applications at the University of Minnesota, Minneapolis, Minnesota, January 12-16, 2009 (invited talk): "Nuclear-Electronic Orbital Approach: Electron-Proton Correlation, Multicomponent Density Functional Theory, and Tunneling Splittings"
175. Gordon Research Conference on Protons and Membrane Reactions, Ventura, California, February 22-27, 2009 (invited talk): "Proton-Coupled Electron Transfer Reactions in Enzymes: Hydrogen Tunneling and Protein Motion"
176. Sanibel Symposium, St. Simons Island, Georgia, February 26- March 3, 2009 (invited talk): "Proton-Coupled Electron Transfer Reactions in Enzymes: Hydrogen Tunneling and Protein Motion"
177. American Chemical Society National Meeting, Symposium entitled Advances in Electronic Structure Theory and First Principles Dynamics, Salt Lake City, Utah, March 22-26, 2009 (invited talk): "Electron-Proton Correlation in the Nuclear-Electronic Orbital Approach: Explicit Correlation and Multicomponent Density Functional Theory"
178. American Chemical Society National Meeting, Symposium entitled Functional Motions in Enzyme Catalysis, Salt Lake City, Utah, March 22-26, 2009 (invited talk): "Proton-Coupled Electron Transfer in Soybean Lipxygenase: 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, Symposium entitled Theory and Applications of Density Functional Theory, San Diego, California, March 25-29, 2012 (invited talk): “Multicomponent Density Functional Theory: Development of Electron-Proton Functionals”
 224. University of Illinois, Urbana-Champaign, Illinois, April 5, 2012 (seminar): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
 225. Arizona State University, Phoenix, Arizona, April 13, 2012 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
 226. MIT and Harvard University, Boston, Massachusetts, April 19, 2012 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
 227. 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 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, 2015 (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 pKa's and Redox Potentials, Boston, Massachusetts, August 16-20, 2015 (invited talk): "Calculating pKa's, Reduction Potentials, and Reorganization Energies for Electrochemical Proton-Coupled Electron Transfer Processes"
289. American Chemical Society National Meeting, Symposium entitled The Role of the Outer Coordination Sphere on the Activity of Enzymes and Molecular Catalysts, Boston, Massachusetts, August 16-20, 2015 (invited talk): "Pendant Proton Relays and Ligand Non-Innocence in Hydrogen-Evolving Molecular Electrocatalysts"
290. American Chemical Society National Meeting, Symposium for the 2015 ACS Catalysis Lectureship for the Advancement of Catalytic Science, Boston, Massachusetts, August 16-20, 2015 (invited talk): "Theoretical Design of Hydrogen-Evolving Molecular Electrocatalysts"
291. Midwest Computational Biomolecular Modeling Symposium, Beckman Institute, University of Illinois. Urbana, Illinois, September 15-16, 2015 (invited talk): "Computational Macromolecular Modeling: Future Directions"
292. University of Minnesota, Energy Frontier Research Center, Minneapolis, Minnesota, October 4, 2016 (invited after dinner talk): "How Centers Make a Difference"
293. University of Minnesota, Minneapolis, Minnesota, October 5, 2016 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
294. Mathematical Biosciences Institute Workshop on Multiple Faces of Biomolecular Electrostatics, Ohio State University, Columbus, Ohio, October 12-16, 2015 (key note talk): "Probing Electrostatics and Conformational Motions in Enzyme Catalysis"
295. Georgia Institute of Technology, Atlanta, Georgia, November 2, 2015 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
296. Emory University, Atlanta, Georgia, November 3, 2015 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
297. Yale University, Symposium for John Tully, New Haven, Connecticut, November 7, 2015 (invited talk): "Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer Processes"

298. Pacifichem 2015, Symposium entitled Recent Progress in Molecular Theory for Excited-State Electronic Structure and Dynamics, Honolulu, Hawaii, December 15-20, 2015 (invited talk): "Photoinduced Proton-Coupled Electron Transfer in Solution: Quantum Mechanical/Molecular Mechanical Nonadiabatic Dynamics"
299. Pacifichem 2015, Symposium entitled Molecular Catalysis of Water Splitting Reactions, Honolulu, Hawaii, December 15-20, 2015 (invited talk): "Theoretical Design of Hydrogen-Evolving Molecular Electrocatalysts"
300. Pacifichem 2015, Symposium entitled Dynamical Intermolecular Interactions for Biological Functions, Honolulu, Hawaii, December 15-20, 2015 (invited talk): "Probing Electrostatics and Conformational Motions along the Catalytic Cycle of an Enzyme"
301. Gordon Research Conference on Electrochemistry, Ventura, California, January 10-15, 2016 (invited talk): "Theoretical Design of Hydrogen-Evolving Molecular Electrocatalysts"
302. University of California at Los Angeles, Los Angeles, California, January 13, 2016 (Distinguished Lecture): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
303. Jean Dreyfus Boissevain Lectureship, University of Colorado at Denver, Denver, Colorado, March 9, 2016 (invited named lecture): "Enzymes: The Engines of Biology"
304. Jean Dreyfus Boissevain Lectureship, University of Colorado at Denver, Denver, Colorado, March 10, 2016 (invited public lecture): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
305. University of Colorado, Boulder, Colorado, March 11, 2016 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
306. National Plenary Lecture at American Chemical Society National Meeting, San Diego, California, March 13-17, 2016 (invited National Lecture): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
307. American Chemical Society National Meeting, Symposium entitled Computational Enzymology, San Diego, California, March 13-17, 2016 (invited talk): "Probing Electrostatics and Conformational Motions along the Catalytic Cycle of Dihydrofolate Reductase"
308. American Chemical Society National Meeting, Symposium entitled Computational Materials Chemistry, San Diego, California, March 13-17, 2016 (invited talk): "Avoiding the Born-Oppenheimer Separation between Electrons and Protons: Explicitly Correlated Wavefunctions and Multicomponent Density Functional Theory"
309. American Chemical Society National Meeting, Symposium entitled Structure and Dynamics in Enzymatic Catalysis across Multiple Timescales: Experiment and Theory, San Diego, California, March 13-17, 2016 (invited talk): "Proton-Coupled Electron Transfer in Soybean Lipoxigenase: Hydrogen Tunneling and Conformational Motions"
310. Walter Kauzmann Lecturer, Princeton University, Princeton, New Jersey, April 18, 2016 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
311. AFOSR Molecular Dynamics Contractor's Meeting, Arlington, Virginia, May 24-26, 2016 (invited talk): "Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer"
312. EMBO Conference entitled The Biochemistry and Chemistry of Biocatalysis: From Understanding to Design, Oulu, Finland, June 12-15, 2016 (invited talk): "Probing Electrostatics and Conformational Motions along the Catalytic Cycle of an Enzyme"
313. Empirical Valence Bond Conference, Uppsala, Sweden, June 23-25, 2016 (invited talk): "Theory of Proton-Coupled Electron Transfer"
314. 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, Massachusetts, July 10-15, 2016 (invited talk): “Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer Processes”
316. Gordon Research Conference on Computational Chemistry, Girona, Spain, July 24-28, 2016 (invited talk): “Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer”
317. American Chemical Society National Meeting, Symposium entitled QM/MM Simulation of Chemical and Biochemical Reaction Pathways: Recent Developments and Applications, Philadelphia, Pennsylvania, August 21-25, 2016 (invited talk): “Mechanistic Strategies in Ribozymes: Catalytic Roles of Metal Ions, Nucleobases, and Cofactors”
318. American Chemical Society National Meeting, Symposium entitled Dynamics of Natural and Artificial Systems for Energy Conversion: Insights Gained from Spectroscopic Methods and Theory, Philadelphia, Pennsylvania, August 21-25, 2016 (invited talk): “Electrochemical and Photoinduced Proton-Coupled Electron Transfer in Energy Conversion Processes”
319. American Chemical Society National Meeting, Symposium entitled Computational Chemistry for Energy Application, Philadelphia, Pennsylvania, August 21-25, 2016 (invited talk): “Theoretical Design of Hydrogen-Evolving Molecular Electrocatalysts”
320. Theory and Applications of Computational Chemistry, Seattle, Washington, August 28 – September 2, 2016 (invited plenary lecture): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
321. Institute for Sustainability, Energy, and Environment (iSEE) Congress 2016 on Energy 2030: Paths to a Sustainable Future, September 12-14, 2016 (invited talk): “Solar Energy through Better Chemistry”
322. Faraday Discussion on Chemical Reaction Rate Theory, Cambridge, United Kingdom, September 19-21, 2016 (invited headline speaker): “Proton-Coupled Electron Transfer Reactions: Analytical Rate Constants and Case Study of Kinetic Isotope Effects in Lipxygenase”
323. Thomas-Young Centre (TYC) for Materials Modelling, London, United Kingdom, September 22, 2016 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
324. University of Bristol, Bristol, United Kingdom, September 23, 2016 (invited talk): “Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer Processes”
325. CIFAR Bio-Inspired Solar Energy Meeting, Montreal, Canada, October 28-29, 2016 (invited talk): “Inspiration from Biology: Coupling Electrons and Protons and Facilitating Tunneling”
326. Brooklyn College, New York, New York, November 22, 2016 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
327. Northeastern University, Boston, Massachusetts, January 18, 2017 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
328. Northwestern University, Evanston, Illinois, February 2, 2017 (invited talk): “Proton-Coupled Electron Transfer in Energy Conversion Processes”
329. Armstrong Lecture, Vanderbilt University, Nashville, Tennessee, February 24, 2017 (named lecture): “Enzyme Catalysis through the Lens of Theory”
330. Brandeis University, Boston, Massachusetts, March 6, 2017 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
331. Greater Boston Area Theoretical Chemistry Lecture, MIT, Harvard, Boston University, Boston, Massachusetts, March 8, 2017 (invited talk): “Proton-Coupled Electron Transfer: Theory and Applications”
332. American Chemical Society National Meeting, Symposium entitled Multicenter Molecules and Coupled Molecular Assemblies – Synthesis, Characterization, and Theory, San Francisco,

- California, April 2-6, 2017 (invited talk): “Theoretical Studies of Homogeneous and Heterogeneous Multicenter Electrocatalysts”
333. American Chemical Society National Meeting, Symposium entitled Light-Driven Chemistry: Photoelectrochemistry and Photocatalysis, San Francisco, California, April 2-6, 2017 (invited talk): “Photoinduced Proton-Coupled Electron Transfer in Solvated Molecular Systems and Photoreceptor Proteins”
334. American Chemical Society National Meeting, Symposium entitled Strong Electron Correlation and Nonadiabatic Dynamics, San Francisco, California, April 2-6, 2017 (invited talk): “Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer Processes”
335. W. A. Noyes Distinguished Lecture, University of Texas at Austin, Austin, Texas, April 20, 2017 (named lecture): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
336. Neckers Lecture, Southern Illinois University, Carbondale, Illinois, May 5, 2017 (named lecture): “Proton-Coupled Electron Transfer: Moving Together and Charging Forward”
337. Chemical Society of Canada, Symposium entitled Quantum Coherence and Dynamics in Biological Systems, Toronto, Canada, May 29-30, 2017 (invited talk): “Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer in Solution and Photoreceptor Proteins”
338. International Academy of Quantum Molecular Science Annual Meeting Anniversary Celebration, session on Future of Quantum Molecular Science, Menton, France, June 30, 2017 (invited talk): “Methods for Integrating Electronic and Nuclear Quantum Effects”
339. 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. Penn Conference in Theoretical Chemistry (PCTC), Philadelphia, Pennsylvania, August 17-19, 2017 (invited talk): “Interfacial Electrochemical Proton-Coupled Electron Transfer”
342. American Chemical Society National Meeting, Washington, DC, August 20-24, 2017, symposium entitled New Paradigm for Catalyst Design: From Enzymatic Function to Functional Mimics (invited talk): “Inspiration from Biology: Coupling Electrons and Protons and Facilitating Tunneling”
343. WATOC, Munich, Germany, August 27-September 1, 2017 (invited talk): “Multicomponent Density Functional Theory: Integrating Electronic and Nuclear Quantum Effects”
344. ACS Publications Symposium entitled Innovation in Energy Conversion – A Physical Chemistry Perspective, Dalian, China, September 24-26, 2017 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
345. Tsinghua University, Beijing, China, September 27, 2017 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
346. Klaus Schulten Memorial Symposium, University of Illinois, Urbana, Illinois, November 7-9, 2017 (invited talk): “Proton-Coupled Electron Transfer in Enzymes and Photoreceptor Proteins”
347. Chemistry and Mathematics in Phase Space (CHAMPS) Meeting, Bristol, United Kingdom, January 15-16, 2018 (invited talk): “Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer Processes”
348. Gordon Research Conference on Metals in Biology, Ventura, California, January 21-26, 2018 (invited talk): “Proton-Coupled Electron Transfer and the Catalytic Role of Iron in Soybean Lipoxygenase”
349. Virginia Tech, Highlands in Chemistry seminar series, Blacksburg, Virginia, March 2, 2018 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”

350. AFOSR Workshop on Chemical Tools for Biological Processes, Dayton, Ohio, March 13, 2018 (invited talk): "Theoretical Perspectives of Proton-Coupled Electron Transfer in Biological Systems"
351. American Chemical Society National Meeting, New Orleans, Louisiana, March 18-22, 2018, symposium entitled Computational Catalyst Design for Energy Conversion and Storage (invited talk): "Theoretical Design of Molecular Electrocatalysts with Proton Relays for Energy Conversion Processes"
352. American Chemical Society National Meeting, New Orleans, Louisiana, March 18-22, 2018, symposium entitled PCET Photocatalysis with Inorganic Molecules and Materials (invited talk): "Proton-Coupled Electron Transfer in Artificial Photosynthesis and Photoreduced Nanoparticles"
353. American Chemical Society National Meeting, New Orleans, Louisiana, March 18-22, 2018, symposium entitled Insights into Structure, Function, Dynamics and Evolution of Enzymatic Mechanisms (invited talk): "Proton-Coupled Electron Transfer in Soybean Lipoxygenase: Hydrogen Tunneling, Electrostatics, and Conformational Motions"
354. American Chemical Society National Meeting, New Orleans, Louisiana, March 18-22, 2018, symposium entitled Awards Symposium for James Mayer (invited talk): "Interfacial Proton-Coupled Electron Transfer: Interplay between Experiment and Theory"
355. American Chemical Society National Meeting, New Orleans, Louisiana, March 18-22, 2018, symposium entitled Awards Symposium for Thomas Rauchfuss (invited talk): "Hydrogen-Evolving Molecular Electrocatalysts: Interplay between Experiment and Theory"
356. American Chemical Society National Meeting, New Orleans, Louisiana, March 18-22, 2018, symposium entitled Dreyfus Awards Symposium (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
357. Nebraska Cluster for Computational Chemistry (NC3) Award Lecture, University of Nebraska-Lincoln, Lincoln, Nebraska, March 30, 2018 (invited award lecture): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
358. Conference on Predictive Catalysis: Transition-Metal Reactivity by Design, Girona, Spain, April 4-6, 2018 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
359. COST Action CM1305 Conference on Explicit Control over Spin States, Berlin, Germany, April 9-11, 2018 (invited talk): "Theoretical Design of Molecular Electrocatalysts for Energy Conversion Processes"
360. Annual Meeting of the American Society of Biochemistry & Molecular Biology (ASBMB), San Diego, California, April 21-25, 2018 (invited talk): "Proton-Coupled Electron Transfer in Soybean Lipoxygenase: Hydrogen Tunneling and Conformational Motions"
361. Annual Yale Science and Engineering Forum, New Haven, Connecticut, May 3, 2018 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
362. University of Pennsylvania, Philadelphia, Pennsylvania, May 9, 2017 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
363. Proton-Coupled Electron Transfer (PCET 2018), Blowing Rock, North Carolina, June 10-14, 2018 (invited talk): "Interfacial Proton-Coupled Electron Transfer: Photoreduced Nanocrystals and Metal Electrodes"
364. Weizmann Institute, Faculty of Chemistry, Lifson Memorial Lecture, Rehovot, Israel, June 18, 2018 (invited named lecture): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
365. Photoinduced Processes in Embedded Systems (PPES 2018), Pisa, Italy, June 24-27, 2018 (invited talk): "Photoinduced Proton-Coupled Electron Transfer: Integrating Electronic and Nuclear Quantum Effects"
366. CCI Solar Fuels Capstone Meeting, Ventura, California, July 8-12, 2018 (invited talk): "Proton-Coupled Electron Transfer: Moving Together and Charging Forward"

367. Telluride workshop on Condensed Phase Dynamics, Telluride, Colorado, July 16-20, 2018 (invited talk): "Recent Advances in the Theory of Proton-Coupled Electron Transfer"
368. Gordon Research Conference on Electron Donor-Acceptor Interactions, Newport, Rhode Island, August 5-10, 2018 (invited talk): "Proton-Coupled Electron Transfer: Moving Together and Charging Forward"
369. American Chemical Society National Meeting, Boston, Massachusetts, August 19-23, 2018, symposium entitled Computational Photocatalysis: Modeling of Photophysics & Photochemistry at Interfaces (plenary talk): "Interfacial Proton-Coupled Electron Transfer: Artificial Photosynthesis and Photoreduced Nanoparticles"
370. Brookhaven National Laboratory, Upton, New York, September 10, 2018 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
371. Pennsylvania State University, University Park, Pennsylvania, October 17, 2018 (colloquium): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
372. Musselman Visiting Scientist and Lecturer, Gettysburg College, Gettysburg, Pennsylvania October 18, 2018 (endowed lecture series): "Enzymes: The Engines of Biology"
373. Musselman Visiting Scientist and Lecturer, Gettysburg College, Gettysburg, Pennsylvania October 18, 2018 (endowed lecture series): "Out of the Beaker and onto the Hard Drive: The Emergence of Theoretical Chemistry"
374. Musselman Visiting Scientist and Lecturer, Gettysburg College, Gettysburg, Pennsylvania October 18, 2018 (endowed lecture series): "Solar Energy through Better Chemistry"
375. Musselman Visiting Scientist and Lecturer, Gettysburg College, Gettysburg, Pennsylvania October 18, 2018 (endowed lecture series): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
376. Connecticut Valley Quantum Chemistry Meeting, Yale University, New Haven, Connecticut, October 31, 2018 (invited talk): "Multicomponent Quantum Chemistry: Integrating Electronic and Nuclear Quantum Effects"
377. Department of Molecular Biophysics and Biophysics, Yale University, New Haven, Connecticut, January 28, 2018 (invited talk): "Proton-Coupled Electron Transfer in Enzymes and Photoreceptor Proteins"
378. G. M. Kosolapoff Award, Auburn University, February 13, 2019 (award talk): "Enzymes: The Engines of Biology"
379. G. M. Kosolapoff Award, Auburn University, February 14, 2019 (colloquium): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
380. Sanibel Symposium, February 17, 2019 (plenary talk): "Multicomponent Quantum Chemistry: Integrating Electronic and Nuclear Quantum Effects"
381. Kenneth S. Pitzer Lecture, University of California at Berkeley, March 19, 2019 (named lecture): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
382. 47th John Stauffer Lecture in the Sciences, University of Southern California, Los Angeles, California, March 21, 2019 (Distinguished Speaker): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
383. 47th John Stauffer Symposium in the Sciences, University of Southern California, Los Angeles, California, March 21, 2019 (Distinguished Speaker): "Multicomponent Quantum Chemistry: Integrating Electronic and Nuclear Quantum Effects"
384. American Chemical Society National Meeting, Orlando, Florida, March 31 – April 4, 2019, Murray Goodman Memorial Prize symposium (invited talk): "Conformational Motions and Electrostatics Facilitate Proton-Coupled Electron Transfer in BLUF Photoreceptor Proteins"

385. American Chemical Society National Meeting, Orlando, Florida, March 31 – April 4, 2019, Harry Gray Award for Creative Work in Inorganic Chemistry symposium (invited talk): “Proton-Coupled Electron Transfer and Driving Force: A Complicated Relationship”
386. Ultrafast Photoinduced Energy and Charge Transfer: Faraday Discussion, Ventura, California, April 8-10, 2019 (headline speaker): “Theoretical Analysis of the Inverted Region in Photoinduced Proton-Coupled Electron Transfer”
387. MURI meeting on Molecular Level Studies of Solid-Liquid Interfaces in Electrochemical Processes, Washington, DC, April 29-30, 2019 (talk): “Proton-Coupled Electron Transfer at Electrochemical Interfaces”
388. 24th John Stauffer Lecturer in Chemistry, Stanford University, Stanford, California, May 14, 2019 (named lecture): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
389. 24th John Stauffer Lecturer in Chemistry, Stanford University, Stanford, California, May 16, 2019 (named lecture) “Multicomponent Quantum Chemistry: Integrating Electronic and Nuclear Quantum Effects”
390. AFOSR Molecular Dynamics/Theoretical Chemistry Program Review, Washington, DC, May 21-23, 2019 (invited talk): “Conformational Motions and Electrostatics Facilitate Proton-Coupled Electron Transfer in BLUF Photoreceptor Proteins”
391. DOE CTC PI Meeting, Gaithersburg, Maryland, May 22-24, 2019 (invited talk): “Multicomponent Quantum Chemistry Methods for Electrons and Nuclei or Positrons”
392. Almlöf–Gropen Lecture, University of Oslo, Oslo, Norway, June 13, 2020 (named lecture): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
393. International Society of Theoretical Chemical Physics (ISTCP), University of Tromsø, Tromsø, Norway, July 11-17, 2019 (opening keynote lecture): “Multicomponent Quantum Chemistry: Integrating Electronic and Nuclear Quantum Effects”
394. Research Workshop on TDDFT – Excitations and Dynamics, Rutgers University, New Brunswick, New Jersey, August 11-14, 2019 (invited talk): “Multicomponent Time-Dependent Density Functional Theory: Integrating Electronic and Vibrational Excitations”
395. American Chemical Society National Meeting, San Diego, California, August 25-29, 2019, symposium entitled Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer (invited talk): “Multicomponent Quantum Chemistry: Integrating Electronic and Nuclear Quantum Effects”
396. American Chemical Society National Meeting, San Diego, California, August 25-29, 2019, symposium entitled Frontiers in Interdisciplinary Research: New Paradigms for Integration of Theory and Experiment (invited talk): “Mechanistic Strategies of Ribozymes and DNA Polymerases”
397. American Chemical Society National Meeting, San Diego, California, August 25-29, 2019, symposium entitled Exploring Transition Metal Chemistry & Spectroscopy with Quantum Chemistry (invited talk): “Interfacial Proton-Coupled Electron Transfer at Nanoparticles and Electrodes Composed of Transition Metals”
398. Faraday Discussion meeting on Quantum Effects in Complex Systems, Warwick, Coventry, United Kingdom, September 11-13, 2019 (Closing Remarks Speaker): “Quantum Effects in Complex Systems: Closing Remarks”
399. Harvard University, Boston, Massachusetts, October 7, 2019 (invited talk, Woodward CCB Departmental Colloquium): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
400. Cornell University, CABES Energy Symposium, Ithaca, New York, October 11, 2019 (invited talk presented remotely): “Interfacial Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”

401. University of Toronto, Toronto, Canada, October 17, 2019 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
402. CIFAR Bio-Inspired Solar Energy Meeting, Toronto, Canada, October 18, 2019 (invited talk): “How Do Enzymes Control Chemical Reactions?”
403. Workshop on Recent Advances in Electron and Proton Transfer Reaction Theories, New York, New York, October 25, 2019 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
404. Jean Dreyfus Lectureship, Georgia Southern University, Statesboro, Georgia, November 14, 2019 (technical talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
405. Jean Dreyfus Lectureship, Georgia Southern University, Savannah, Georgia, November 15, 2019 (public talk): “Enzymes: The Engines of Biology”
406. Johns Hopkins University, Baltimore, Maryland, December 3, 2019 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
407. University of Texas Southwestern, Molecular Biophysics Discussion Group, Dallas, Texas, December 12, 2019 (invited talk): “Proton-Coupled Electron Transfer in Bioinspired and Biological Systems”
408. Wesleyan University, Middletown, Connecticut, January 31, 2020 (colloquium): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
409. Virtual Winter School on Computational Chemistry, February 18, 2020 (invited talk): “Proton-Coupled Electron Transfer: Theoretical Perspectives and Applications”
410. Borden Lecture, University of Washington, Seattle, Washington, February 26, 2020 (named lecture): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
411. University of Göttingen, Germany, June 22, 2020 (invited talk, webinar): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
412. Virtual Conference on Theoretical Chemistry, July 27-29, 2020 (plenary talk, virtual): “Proton-Coupled Electron Transfer: Analytical Theories to Nuclear-Electronic Dynamics”
413. MURI meeting on Molecular Level Studies of Solid-Liquid Interfaces in Electrochemical Processes, August 10, 2020 (talk, virtual): “Interfacial Electric Fields at Electrode Interfaces: Vibrational Probes and Graphite-Conjugated Acids”
414. Warren Group Alumni Seminar Series, August 17, 2020 (invited talk, virtual): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
415. International Society of Electrochemistry Annual Meeting, August 31 – September 1, 2020 (plenary lecture, virtual): “Proton-Coupled Electron Transfer in Electrochemistry”
416. Utah State University, September 9, 2020 (departmental seminar, virtual): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
417. EPFL, October 15, 2020 (invited seminar, virtual): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
418. Caltech Chemical Physics Seminar Series, October 27, 2020 (invited talk, virtual): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
419. Electrochemical Society Webinar Series, October 28, 2020 (invited talk, webinar): “Proton-Coupled Electron Transfer in Electrochemistry”
420. University of Utah, November 9, 2020 (departmental seminar, virtual): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
421. ACS PHYS webinar lecture, November 13, 2020: “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”

422. University of Wisconsin-Eau Claire, November 20, 2020 (seminar, virtual): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
423. Lowdin Lecture, Uppsala, Sweden, December 3-4, 2020 (award talk, virtual): "Multicomponent Quantum Chemistry: Integrating Electronic and Nuclear Quantum Effects via the Nuclear-Electronic Orbital Method"
424. Free University Berlin, December 9, 2020 (seminar, virtual): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
425. Stony Brook University, Stony Brook, New York, January 29, 2021 (seminar, virtual): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
426. University of Hong Kong, February 2, 2021 (seminar, virtual): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
427. New Jersey Institute of Technology, Newark, New Jersey, February 3, 2021 (seminar, virtual): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
428. Virtual Winter School on Computational Chemistry, February 15, 2021 (invited talk): "Multicomponent Quantum Chemistry: Integrating Electronic and Nuclear Quantum Effects"
429. West Chester University, West Chester, Pennsylvania, February 22, 2021 (seminar, virtual): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
430. Rutgers University, Department of Chemistry and Chemical Biology, February 23, 2021 (invited talk, virtual): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
431. University of Oxford, United Kingdom, March 1, 2021 (invited seminar, virtual): "Theoretical Perspectives on Proton-Coupled Electron Transfer"
432. Faraday Joint Interest Group Conference, Sheffield, UK, March 29-31, 2021 (plenary talk, virtual): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
433. Condon Lecture, University of Colorado, Boulder, April 2, 2021 (named lecture, virtual): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
434. American Chemical Society meeting, PHYS Awards Symposium, April 5-16, 2021 (award lecture, virtual): "Theoretical Perspectives on Proton-Coupled Electron Transfer"
435. American Chemical Society meeting, Symposium on Dynamics of Chemical Reactions from Gas Phase to Interfaces, April 5-16, 2021 (invited talk, virtual): "Multicomponent Quantum Chemistry: Integrating Electronic and Nuclear Quantum Effects"
436. Fritz-Haber-Institute of the Max-Planck Society, Seminar of the Theory Department, Berlin, Germany, April 22, 2021 (invited talk, virtual): "Theoretical Perspectives on Proton-Coupled Electron Transfer"
437. AFOSR Molecular Dynamics and Theoretical Chemistry Program Review, May 25-27, 2021 (invited talk, virtual): "Heterogeneous Electrochemical Proton-Coupled Electron Transfer"
438. Psi-k workshop on Principles of Light-Induced Charge Transfer for Optogenetics, June 14-16, 2021 (invited talk, virtual): "Nonequilibrium Excited State Dynamics of Proton-Coupled Electron Transfer in BLUF Photoreceptor Proteins"
439. CECAM workshop on Nonequilibrium Dynamical Solvent Effects on Excited States: From Spectroscopy to Photoreactivity, June 14-17, 2021 (invited talk, virtual): "Nonequilibrium Dynamics of Photoinduced Proton-Coupled Electron Transfer in Solution and Photoreceptor Proteins"
440. Telluride workshop on Proton Transfer in Biology, Telluride, Colorado, June 22-26, 2021 (invited talk, virtual): "Proton-Coupled Electron Transfer in BLUF Photoreceptor Proteins and Ribonucleotide Reductase"

441. Telluride workshop on Quantum Effects in Condensed-Phase Systems, Telluride, Colorado, June 29 - July 2, 2021 (invited talk, virtual): "Multicomponent Quantum Chemistry: Integrating Electronic and Nuclear Quantum Effects"
442. CompChem UBO seminar, Universidad Bernardo O'Higgins, Chile, July 14, 2021 (invited talk, virtual): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
443. American Chemical Society National Meeting, Atlanta, Georgia, August 22-26, 2021, symposium entitled Orbital Models in Electronic Structure Theory (invited talk, virtual): "Electronic and Protonic Orbitals in Multicomponent Quantum Chemistry"
444. American Chemical Society National Meeting, Atlanta, Georgia, August 22-26, 2021, symposium entitled Synthesizing Quantum Coherence (invited talk, virtual): "Controlling the Pathways for Protons and Electrons"
445. American Chemical Society National Meeting, Atlanta, Georgia, August 22-26, 2021, symposium entitled Synthesizing Quantum Coherence (invited talk, virtual): "Nuclear-electronic orbital methods in quantum chemistry"
446. American Chemical Society National Meeting, Atlanta, Georgia, August 22-26, 2021, symposium entitled Synthesizing Quantum Coherence (invited talk, virtual): "Electron and proton transfer: Coupling together and to my career"
447. Joseph O. Hirschfelder Prize in Theoretical Chemistry, University of Wisconsin, Madison, Wisconsin, September 14, 2021 (general departmental lecture): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
448. Joseph O. Hirschfelder Prize in Theoretical Chemistry, University of Wisconsin, Madison, Wisconsin, September 15, 2021 (research lecture): "Integrating Electronic and Nuclear Quantum Effects via the Nuclear-Electronic Orbital Approach"
449. Gibbs Award Ceremony, Chicago, Illinois, September 17, 2021 (award talk, virtual): "Proton-Coupled Electron Transfer in Chemistry and Biology"
450. Wayne State University, Detroit, Michigan, September 22, 2021 (invited talk, virtual): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
451. TIMB3 Symposium, Lisbon, Portugal, October 1, 2021 (invited talk, virtual): "Proton-Coupled Electron Transfer in Enzymes and Photoreceptor Proteins"
452. NWO CHAINS (Dutch Research Council, Chemistry as Innovating Science) 2021, Veldhoven, Netherlands, December 7-8, 2021 (keynote talk, virtual): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
453. Pacifichem, Honolulu, Hawaii, December 16-21, 2021 (invited talk, virtual): "Proton-Coupled Electron Transfer and Driving Force: A Complicated Relationship"
454. Pacifichem, Honolulu, Hawaii, December 16-21, 2021 (invited talk, virtual): "Nonequilibrium Excited State Dynamics of Proton-Coupled Electron Transfer in BLUF Photoreceptor Proteins"
455. Big Quantum Bio meeting, January 13, 2022 (invited talk, virtual): "Proton-Coupled Electron Transfer in Enzymes and Photoreceptor Proteins"
456. American Physical Society meeting, March 16, 2022 (invited talk, virtual): "Integrating Electronic and Nuclear Quantum Effects via the Nuclear-Electronic Orbital Approach"
457. Electrochemical Online Colloquium, March 17, 2022 (invited talk): "Theoretical Modeling of Electrochemical Proton-Coupled Electron Transfer"
458. American Chemical Society meeting, San Diego, California, symposium entitled Kinetic and Mechanistic Insights into Heterogeneous Catalysis: Theoretical and Experimental Approaches to Catalyst Development, March 20-24, 2022 (invited talk): "Heterogeneous Proton-Coupled Electron Transfer"

459. American Chemical Society meeting, San Diego, California, symposium entitled The Role of Fundamental Interfacial Processes in Electrocatalysis: Fundamental Elements of Electrocatalysis, March 20-24, 2022 (invited talk): "Theory of Proton Discharge on Metal Electrodes"
460. Gordon Research Conference on Photosensory Receptors and Signal Transduction, Ventura, California, March 27 – April 1, 2022 (invited talk): "Nonequilibrium Excited State Dynamics of Proton-Coupled Electron Transfer in BLUF Photoreceptor Proteins"
461. Tufts University, Medford, Massachusetts, April 6, 2022 (invited talk, virtual): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
462. Annual Seminar in Physical Chemistry, Purdue University, April 7, 2022 (invited talk, virtual): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
463. Seymour Rothchild Memorial Lecturer, University of Rochester, April 13, 2022 (named lecture): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
464. Emerson Center Lecture, Emerson University, Atlanta, Georgia, April 21, 2022 (award lecture): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
465. 10th Molecular Quantum Mechanics Conference, Blacksburg, Virginia, June 26 – July 1, 2022 (plenary talk): "Non-Born-Oppenheimer Quantum Dynamics via the Nuclear-Electronic Orbital Approach"
466. Royal Australian Chemical Institute National Congress 2022, Brisbane, Australia, July 3-8, 2022 (plenary talk, virtual): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
467. World Association of Theoretical and Computational Chemists (WATOC), Vancouver, Canada, July 3-8, 2022 (plenary talk): "Integrating Electronic and Nuclear Quantum Effects via the Nuclear-Electronic Orbital Approach"
468. American Conference on Theoretical Chemistry, Squaw Valley, California, July 25-28, 2022 (invited talk): "Photoinduced Proton-Coupled Electron and Energy Transfer"
469. Gordon Research Conference on Vibrational Spectroscopy, Smithfield, Rhode Island, July 31 – August 5, 2022 (invited talk): "Photoinduced Proton-Coupled Electron and Energy Transfer"
470. American Chemical Society National Meeting, symposium entitled Quantum Chemistry: Current and Future Frontiers, Chicago, Illinois, August 21-25, 2022 (invited talk): "Recent Advances in the Nuclear-Electronic Orbital Approach"
471. American Chemical Society National Meeting, symposium entitled Spectroscopy, Imaging, and Dynamics of Energy Related Materials, Chicago, Illinois, August 21-25, 2022, (invited talk): "Interfacial Proton-Coupled Electron Transfer"
472. CECAM workshop on Theories of Molecular Processes and Spectra based on the Quantum-Classical Synergy, Bordeaux, France, September 5-7, 2022 (invited talk, virtual): "Non-Born-Oppenheimer Quantum Dynamics via the Nuclear-Electronic Orbital Approach"
473. Judith Klinman 80th+ Symposium, Boston, Massachusetts, September 17, 2022 (invited talk): "Proton-Coupled Electron Transfer in Enzymes and Photoreceptor Proteins"
474. Inaugural NYU Simons Center for Computational Physical Chemistry Symposium, New York University, New York, New York, October 7, 2022 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
475. Symposium on Solvation Science, Cluster of Excellence RESOLV, Ruhr-Universität Bochum, Bochum, Germany, November 3-4, 2022 (invited talk): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
476. Uppsala University, Uppsala Sweden, December 1, 2022 (general seminar): "Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"

477. Löwdin Lecture, Uppsala University, Uppsala, Sweden, December 2, 2022 (named lecture):
“Integrating Electronic and Nuclear Quantum Effects via the Nuclear-Electronic Orbital Approach”
478. Gordon Research Conference on Inorganic Reaction Mechanisms, Galveston, Texas, March 5-10, 2023 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
479. Gordon Research Conference on Quantum Biology, Galveston, Texas, March 19-23, 2023 (invited talk): “Proton-Coupled Electron Transfer in Enzymes and Photoreceptor Proteins”
480. American Chemical Society National Meeting, symposium entitled Charge Transfer and Energy Conversion at Interfaces and Defects, Indianapolis, Indiana, March 26-30, 2023 (invited talk):
“Proton-Coupled Electron and Energy Transfer Processes”
481. American Chemical Society National Meeting, symposium entitled A Solar Fuels Nexus: Molecules and Materials for Light-Driven Catalysis, Indianapolis, Indiana, March 28, 2023 (invited talk):
“Proton-Coupled Electron Transfer in Solar Energy Conversion”
482. American Chemical Society National Meeting, symposium entitled ACS Award for Computers in Chemical & Pharmaceutical Research in Honor of Jiali Gao, Indianapolis, Indiana, March 28, 2023 (invited talk): “Integrating Electronic and Nuclear Quantum Effects via the Nuclear-Electronic Orbital Approach”
483. Eastern Regional Photosynthesis Conference, Woods Hole, Massachusetts, April 14-16, 2023 (invited talk): “Proton-Coupled Electron Transfer Relevant to Photosynthesis”
484. Virtual workshop entitled Time-Resolved Spectroscopy Meets Time-Resolved Crystallography: The Future of Dynamic Photobiology, April 17-19, 2023 (invited talk): “Nonequilibrium Excited State Dynamics of Proton-Coupled Electron Transfer in BLUF Photoreceptor Proteins”
485. Northwestern University, Evanston, Illinois, May 3, 2023 (departmental seminar): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
486. Rice-Berry Lecture, University of Chicago, Chicago, Illinois, May 5, 2023 (named lecture): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
487. 243rd Meeting of The Electrochemical Society, Boston, Massachusetts, May 28-June 2, 2023 (keynote lecture): “Electrochemical Proton-Coupled Electron Transfer Theory”
488. 4th International Conference on Proton-Coupled Electron Transfer (PCET), Port Aventura, Spain, June 5-9, 2023 (invited talk): “Hydrogen Tunneling and Excited Vibronic States in Proton-Coupled Electron Transfer”
489. Simons Center International Workshop on Nuclear Quantum Effects in Chemistry, New York University, New York, New York, June 12-14, 2023 (invited talk): “Integrating Electronic and Nuclear Quantum Effects via the Nuclear-Electronic Orbital Approach”
490. Quantum Effects in Biological Systems (QuEBS), Surrey, United Kingdom, June 26-30, 2023 (keynote speaker): “Proton-Coupled Electron Transfer in Enzymes and Photoreceptor Proteins”
491. CECAM Workshop on Principles of Light-Induced Charge Transfer for Optogenetics, Modena, Italy, July 3-5, 2023 (virtual invited talk) “Nonequilibrium Excited State Dynamics of Proton-Coupled Electron Transfer in BLUF Photoreceptor Proteins”
492. BPS Conference, Proton Reactions: From Basic Science to Biomedical Applications, Tahoe, California, August 20-24, 2023 (invited talk): “Proton-Coupled Electron Transfer in Proteins”
493. Oklahoma State University, Stillwater, Oklahoma, September 7, 2023 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
494. Distinguished Karcher-Barton Awardee Lecture, University of Oklahoma, Norman, Oklahoma, September 8, 2023 (named lecture): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”

495. Science Faculty Distinguished Lecture, University of Hong Kong, October 13, 2023 (invited talk): “Electrochemical and Photochemical Proton-Coupled Electron Transfer”
496. Future Science Week co-organized by Future Forum and Hong Kong Academy of Sciences, Hong Kong, October 15, 2023 (keynote lecture): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
497. Case Western Reserve University, Cleveland, Ohio, November 9, 2023 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
498. Washington University Marcus Lecture, St. Louis, Missouri, November 10, 2023 (named lecture): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
499. KAIST Emerging Materials Symposium, Daejeon, South Korea, November 14, 2023 (invited talk, virtual): “Electrochemical Proton-Coupled Electron Transfer”
500. Enzyme Mechanisms Conference, Naples, Florida, January 3-7, 2024 (invited talk): “Proton-Coupled Electron Transfer in Enzymes”
501. Gordon Research Conference on Renewable Energy: Solar Fuels, Ventura, California, February 4-9, 2024 (invited talk): “Interfacial Proton-Coupled Electron Transfer”
502. University of California at Santa Barbara, Santa Barbara, California, February 10, 2024 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”

Scheduled Talks and Seminars

503. Texas A&M University, Frontiers in Chemical Research seminar, February 26, 2024 (invited talk): “Proton-Coupled Electron Transfer in Catalysis and Energy Conversion”
504. Texas A&M University, Frontiers in Chemical Research seminar, February 27, 2024 (invited talk): “Proton-Coupled Electron Transfer in Enzymes and Photoreceptor Proteins”
505. Texas A&M University, Frontiers in Chemical Research seminar, February 28, 2024 (invited talk): “Integrating Electronic and Nuclear Quantum Effects via the Nuclear-Electronic Orbital Approach”
506. American Physical Society Meeting, symposium on Hydrogen Bonding Interactions and Dynamics, Minneapolis, Minnesota, March 6, 2024 (invited talk): “Impact of Hydrogen Bonding on Proton-Coupled Electron Transfer”
507. American Chemical Society Meeting, symposium entitled In Honor of Gregory Voth’s 65th Birthday: From Quantum Dynamics to Ultra Coarse-Graining, and Everything in Between, New Orleans, Louisiana, March 17-21, 2024 (invited talk): “Real-Time Nuclear-Electronic Orbital Quantum Dynamics”
508. American Chemical Society Meeting, symposium entitled Henry Storch Award Symposium for Prashant Kamat, New Orleans, Louisiana, March 17-21, 2024 (invited talk): “Heterogeneous Proton-Coupled Electron Transfer in Energy Conversion Processes”
509. American Chemical Society Meeting, symposium entitled Crossroads of Thermo-, Electro-, and Photochemical Catalysis, New Orleans, Louisiana, March 17-21, 2024 (invited talk): “Interfacial Electric Fields at Electrode Surfaces: Vibrational Probes and Electrocatalysis”
510. Arthur William Davidson Lecture, University of Kansas, Lawrence, Kansas, April 4-5, 2024 (two invited named lectures)
511. CUNY Advanced Science Research Center, Biochemistry, Biophysics & Biodesign Seminar Series, New York, New York, April 17, 2024 (invited talk): “Proton-Coupled Electron Transfer in Enzymes and Photoreceptor Proteins”
512. Massachusetts Institute of Technology, AD Little Lectureship, Cambridge, Massachusetts, May 7, 2024 (named lecture, general inter-departmental)

513. Massachusetts Institute of Technology, AD Little Lectureship, Cambridge, Massachusetts, May 8, 2024 (named lecture, physical chemistry)
514. 4th International Conference on Hydrogen Atom Transfer (iCHAT 2024), Rome, Italy, June 9-13, 2024 (invited talk)
515. Gordon Research Conference on Molecular Interactions and Dynamics, Stonehill College, Easton, Massachusetts, July 7-12, 2024 (invited talk)
516. Gordon Research Conference on Electron Donor-Acceptor Interactions, Salve Regina University, Newport, Rhode Island, July 28 – August 2, 2024 (invited talk)
517. Symposium on Protonation Dynamics in Protein Function, Freie Universität, Berlin, Germany, September 1-3, 2024 (keynote speaker)

Teaching

University of Notre Dame

Chem 647: Computer Simulation of Organic and Biological Systems
Fall 1995, Fall 1996, Fall 1997
Chem 643: Seminar in Physical Chemistry
Fall 1996, Spring 1997, and Fall 1997
Chem 649: Quantum Mechanics
Spring 1997, Spring 1998
Chem 321: Physical Chemistry I (undergraduate thermodynamics and kinetics)
Fall 1999
Chem 322: Physical Chemistry II (undergraduate quantum mechanics)
Spring 2000

Penn State University

Chem 454/565: Introduction to Quantum Chemistry/Quantum Chemistry I
(advanced undergraduate and graduate quantum mechanics)
Fall 2000, 2002, 2003, 2004, 2005
Chem 452: Physical Chemistry II (undergraduate quantum mechanics and kinetics)
Fall 2001
Chem 451: Physical Chemistry I (undergraduate thermodynamics)
Fall 2006
Chem 450: Physical Chemistry I (undergraduate thermodynamics)
Fall 2007
Chem 464: Chemical Kinetics and Dynamics (advanced undergraduate course)
Fall 2009, Fall 2010, Fall 2011

University of Illinois

Chem 442, Introduction to Quantum Chemistry
(undergraduate quantum mechanics)
Fall 2013, Fall 2014, Fall 2015, Fall 2016, Fall 2017
Chem 550: Advanced Quantum Dynamics
Spring 2014

Yale University

Chem 470/570, Quantum Chemistry
combined advanced undergraduate and graduate course
Fall 2018, 2019, 2020
Chem 426/526, Computational Chemistry and Biochemistry
combined undergraduate and graduate course
Spring 2019, 2020, 2022
Chem 466/566 and 467/567, Introduction to Quantum Chemistry I and II
Fall 2021, Fall 2022, Fall 2023
Chem 496/596, Computational Quantum Chemistry
Spring 2022, Spring 2023

Outreach and Education

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

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

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

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

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

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

Designed and created a web site on proton-coupled electron transfer (PCET) reactions, which are central in a wide range of chemical and biological processes, including energy conversion processes. The web site is open to the public at <http://webpcet.chem.yale.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.

Founded and developed the nuclear-electronic orbital (NEO) method for the inclusion of nuclear quantum effects in electronic structure calculations and incorporated this method into several different quantum chemistry packages, including GAMESS, Q-Chem, FHI-aims, and Quantum Chronus.

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