

# TODD J. MARTINEZ



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Todd.Martinez@stanford.edu



**PERSONAL** Born March 22, 1968

## EDUCATION

Postdoctoral Scholar, University of California, Los Angeles and Hebrew University, Jerusalem, Israel	1994-1996
Postdoctoral Advisor: Raphael D. Levine	
PhD in Physical Chemistry, University of California, Los Angeles	1994
Doctoral Advisor: Emily A. Carter	
Dissertation topic: <i>Pseudospectral Treatments of Electron Correlation</i>	
BS in Chemistry, Calvin College, Grand Rapids, MI	1989

## ACADEMIC APPOINTMENTS

D. M. Ehrsam and E. C. Franklin Professor, Stanford University	2009-present
Professor of Photon Science, SLAC National Accelerator Laboratory	2009-present
Professor of Chemistry, Stanford University	2009-present
Edward William and Jane Marr Gutgsell Chair in Chemistry, UIUC	2006-2008
Visiting Professor, Ecole Normal Superieure, Paris, France	2006
Professor of Chemistry, UIUC	2004-2009
Associate Professor of Chemistry, UIUC	2002-2004
Faculty Member, UIUC Center for Biophysics and Computational Biology	2000-2008
Affiliate, Beckman Institute for Advanced Science and Technology	1996-2008
Assistant Professor of Chemistry, UIUC	1996-2002

## HONORS AND AWARDS

Elected Member, National Academy of Sciences	2019
Elected Member, International Academy of Quantum Molecular Science	2017
IAS Benjamin Meaker Visiting Professor, University of Bristol	2017
Elected Fellow, American Academy of Arts and Sciences	2011
National Security Science and Engineering Faculty Fellow (NSSEFF)	2010
Distinguished Alumnus, Carol Morgan School, Dominican Republic	2008
AAAS Fellow, American Association for the Advancement of Science	2006
APS Fellow, American Physical Society	2005
MacArthur Fellow, John D. and Catherine T. MacArthur Foundation	2005
UIUC Excellent Teacher	2005
NSF Special Creativity Extension	2004
UIUC University Scholar	2004
Helen Corley Petit Professor, UIUC College of Liberal Arts and Sciences	2002
UIUC School of Chemical Sciences Excellence in Teaching Award	2001
Teacher Scholar Award, Camille and Henry Dreyfus Foundation	2000
Beckman Fellow, UIUC Center for Advanced Study	2000
Packard Fellow, David and Lucille Packard Foundation	1999
Beckman Young Investigator, Beckman Foundation	1999
Sloan Fellow, Sloan Foundation	1999

Research Innovation Award, Research Corporation	1998
NSF CAREER Award	1998
President's Postdoctoral Fellow, University of California	1994
Fulbright Postdoctoral Fellow	1995
UCLA Excellence in Research Award	1992
NSF Minority Graduate Assistantship	1991
Patricia Harris Roberts Graduate Fellowship	1989

## GRANTS RECEIVED

Except for the MRI, only funds allocated to Martínez research are shown (including indirect costs).

Office of Naval Research MURI, 2018-2023	\$1,250,000
<i>Photomechanical Material Systems – From Molecules to Devices</i>	
(w/R. Hayward, C. Bardeen, J. Read de Alaniz, P. Palffy-Muhoray, and K. Bhattacharya)	
Office of Naval Research MURI, 2018-2023	\$2,000,000
<i>Synthesis Planning and Reaction Discovery for Photochemistry and Chemistry in Novel Environments</i>	
(w/M. Kanan, N. Burns, A. Aspuru-Guzik, S. Lopez, and S. Bradforth)	
National Science Foundation, 2017-2022	\$400,000
<i>Collaborative Research: Systematic Investigation of the Structure, Dynamics, and Energetics of Hydrogen Bonds and the Protein Interior Using Ketosteroid Isomerase and Model Systems</i>	
(w/D. Herschlag)	
Office of Naval Research, 2017-2020	\$750,000
<i>Uncovering Complex Reaction Networks from First Principles</i>	
Department of Energy, 2017-2021	\$1,600,000
<i>SciDAC: Designing Photocatalysts Through Scalable Quantum Mechanics and Dynamics</i>	
(w/A. Aiken, K. Olokotun, L. Ying, P. Huang, T. J. Lane, and H. van den Bedem)	
National Science Foundation, 2017-2020	\$300,000
<i>CCI Phase I: Center for First Principles Design of Quantum Processes</i>	
(w/S. Boxer, T. Markland, M. Fayer, M. Tuckerman, K. Gaffney, and G. Schlau-Cohen)	
National Science Foundation, 2016-2019	\$450,000
<i>Tensor Hypercontraction for Electronic Structure and First Principles Molecular Dynamics</i>	
Global Climate and Energy Project, 2015-2018	\$330,000
<i>Carbonate-Catalyzed CO<sub>2</sub> Hydrogenation to Multi-Carbon Products</i>	
(w/M. Kanan)	
National Science Foundation, 2015-2016	\$112,500
<i>STTR Phase I: An intuitive and tactile quantum mechanical molecular modeling tool for instruction of chemistry students</i>	
(w/J. Quenneville, Spectral Sciences)	
National Science Foundation, 2015-2019	\$600,000
<i>Removing Bottlenecks in High Performance Computational Science</i>	
(w/M. Gordon, T. Windus, L. Slipchenko and T. D. Crawford)	
National Science Foundation, 2014-2017	\$3,500,000
<i>MRI: Acquisition of an Extreme GPU Cluster for Interdisciplinary Research</i>	
(w/V. Pande, M. Gerritsen, and T. Abel – this grant funds a computing resource that will be used by both Stanford and national users)	

Office of Naval Research /AFOSR, 2014-2017 <i>Uncovering Complex Reaction Networks from First Principles</i>	\$850,000
Office of Naval Research MURI, 2012-2017 <i>Shock Wave Energy Dissipation</i> (w/D. Dlott, K. Suslick, J. Moore, N. Sottos, A. Strachan)	\$1,000,000
Department of Energy, 2012-2015 <i>Ultrafast Theory and Simulation</i>	\$1,496,520
Department of Energy, 2012-2015 <i>Predictive Theory of Transition Metal Oxide Catalysts</i> (w/J. Norskov, T. Deveraux, C. Campbell, A. Nilsson)	\$500,000
Army Research Office, 2012-2013 <i>Mechanically Trapping Transition States and Reactive Intermediates</i> (w/S. Craig, S. Sheiko)	\$200,000
National Science Foundation, 2011-2014 <i>International Collaboration in Chemistry: New First Principles Methods for Nonadiabatic Dynamics</i>	\$420,000
Department of Energy, 2009-2012 <i>Attosecond Electron Dynamics</i> (w/P. Bucksbaum, M. Guehr)	\$450,000
Department of Energy, 2009-2012 <i>Strong-Field Control of Molecules</i> (w/P. Bucksbaum, M. Guehr)	\$1,077,000
National Science Foundation, 2010-2014 <i>Collaborative Research: SI2-SSI: Developments in High Performance Electronic Structure Theory</i> (w/M. Gordon, M. Sosonkina, T. Windus, and E. Valeev)	\$800,000
Department of Defense, 2010-2015 <i>Computational and Theoretical Design of Photo- and Mechano-Responsive Molecular Devices</i>	\$3,650,000
Air Force Office of Scientific Research (through Spectral Sciences), 2010-2011 <i>TDDFT on Graphical Processing Units for Modeling Optical Response in Materials</i>	\$45,000
Office of Naval Research, 2009-2010 <i>Novel Multiscale QM/MM Descriptions of Molecular Dynamics Including Charge Transfer</i>	\$110,000
National Science Foundation, 2007-2010 <i>Ab Initio Multiple Spawning Dynamics</i>	\$410,000
Army Research Office, 2007-2012 <i>Mechanochemically-Active Polymer Composites</i> (w/J. Moore, N. Sottos, P. Braun, C. Bielawski and S. Craig)	\$1,000,000
National Science Foundation, 2006-2011 <i>Chemical Computations on Future High-end Computers</i> (w/T. Dunning, R. Pennington, and others)	\$250,000
Department of Energy, Frederick Seitz Materials Research Laboratory, 2005-2006 <i>Nano-Oxide Materials for Photocatalysis and Remediation</i> (w/A. Gewirth, K. Suslick, and others)	\$120,000
Human Frontiers Science Program, 2006-2009 <i>Redesigning Photoactive Proteins in a Tightly Coupled Theoretical and Experimental Feedback Loop</i>	\$350,000

(w/R. van Grondelle and K. Hellingwerf, Amsterdam)	
John D. and Catherine T. MacArthur Foundation, 2005-2010	\$500,000
National Science Foundation, 2005-2008	\$1,000,000
<i>Tools for Ab Initio Molecular Dynamics and Simulation Analysis</i>	
(w/M. Gordon, R. Kendall, M. Sosonkina, and B. Bode)	
Department of Energy, 2005-2008	\$200,000
<i>Cathode Catalysis in Hydrogen/Oxygen Fuel Cells</i>	
(w/A. Gewirth, R. Nuzzo, T. Rauchfuss, A. Wieckowski, and P. Kenis)	
National Science Foundation, 2005-2007	\$235,000
<i>Ab Initio Multiple Spawning Dynamics: Creativity Extension</i>	
Department of Energy, Frederick Seitz Materials Research Laboratory, 2004-2005	\$100,000
<i>Charge Flow in Multiresolution Models of Electron Transfer</i>	
National Science Foundation, 2004-2006	\$125,000
<i>NER: Computational Design of Bio-Opto-Electronic Nanosystems</i>	
National Science Foundation, 2003-2008	\$250,000
<i>ITR: Materials Computation Center</i>	
(w/D. Johnson, R. Martin, D. Ceperley, and others)	
National Science Foundation, 2002-2005	\$331,000
<i>Ab Initio Multiple Spawning Dynamics</i>	
Department of Energy, 2001-2005	\$180,000
<i>A Combined Synthetic, Spectroscopic and Theoretical Approach to the Rational Design of Photophysical and Photochemical Properties of Dendrimers</i>	
(w/C. Bardeen and J. Moore)	
National Science Foundation, 2000-2003	\$60,000
<i>Materials Computation Center</i>	
(w/D. Johnson, R. Martin, D. Ceperley, and others)	
Dreyfus Foundation, 2000-2005	\$50,000
Packard Foundation, 1999-2005	\$625,000
<i>Ab Initio Quantum Photodynamics of Organic and Inorganic Molecules</i>	
Beckman Foundation, 1999-2002	\$200,000
<i>First-Principles Quantum Reaction Dynamics for Ground and Excited Electronic States</i>	
Sloan Foundation, 1999-2001	\$35,000
<i>First-Principles Quantum Reaction Dynamics</i>	
Research Corporation, 1998	\$30,000
<i>Ab Initio Molecular Dynamics of Coupled Electron/Proton Transfer</i>	
National Science Foundation, 1998-2002	\$340,000
<i>Nonadiabatic Effects on Chemical Reaction Dynamics in Gas and Condensed Phases</i>	
UIUC Research Board, 1997	\$24,370
<i>New Methods for Electronic Structure with Photochemical Applications</i>	
National Institutes of Health, 1997-2002	\$280,000
<i>Concurrent Biological Computing</i>	
(w/K. Schulten, R. Skeel, and L. Kale)	
Department of Energy, 1997-2002	\$170,000
<i>Center for Simulation of Advanced Rockets</i>	
(w/M. Heath and others)	

**GRADUATE STUDENTS SUPERVISED**

2017-	K. Grace Johnson	
2017-	Chey Jones	
2017-	Hayley Weir	
2015-	Jimmy Yu	
2015-2017	Laszlo Seress	(MS, 2017; D.E. Shaw Finance, NY)
2015-	David Sanchez	
2015-	Jason Ford	
2015-	Stefan Seritan	
2013-2016	Lin Fan	(MS, 2016; PhD Candidate in Mech. Eng., Stanford)
2013-2015	Nicholas Settje	(MS, 2015; Forward Loop, Hong Kong)
2012-2017	James Snyder	(PhD, 2017; Adobe, CA)
2012-2018	Chenchen Song	(PhD, 2018; Postdoctoral, UC Berkeley)
2011-2016	Aaron Sisto	(PhD, 2016; In-Q-Tel, VA)
2011-2013	Brendan Mar	(MS, 2013)
2011-2016	Sara Kokkila	(PhD, 2016; Postdoctoral, IBM Research, CA)
2011-2017	Fang Liu	(PhD, 2017; Postdoctoral, MIT, MA)
2011-2019	Sofia Izmailov	(PhD, 2019; Data Scientist, Edison Software, CA)
2010-2016	Nicholas Ward	(PhD, 2016; Taipei American School, Taiwan)
2010-2015	Nathan Luehr	(PhD, 2015; Nvidia Corp., CA)
2007-2011	Ivan Ufimtsev	(PhD, 2011; Postdoctoral, Stanford)
2007-2012	Lee Cremar	(PhD, 2012; UT Rio Grande Valley)
2006-2011	Hongli Tao	(PhD, 2011; Lattice Engines, CA)
2005-2009	Jiahao Chen	(PhD, 2009; Data Scientist, Capital One, NY)
2005-2010	Mitchell Ong	(PhD, 2010; Postdoctoral, Livermore National Lab)
2005-2009	Aaron Virshup	(PhD, 2009; Sr Computational Scientist, Arzeda, WA)
2004-2006	Kristina Lamothe	(MS Biophysics, 2006; Early Childhood Program Teacher, MI)
2004-2008	Hanelli Hudock	(PhD, 2008; Vice President, Product Management, ADP, NY)
2003-2009	Chutintorn Punwong	(PhD, 2009; Asst Prof, Prince of Songkla U, Thailand)
2002-2008	Alexis Thompson	(PhD, 2008; Graduate College, UIUC)
2002-2007	Benjamin Levine	(PhD, 2007; Assoc. Prof, Michigan State)
2002-2008	Chaehyuk Ko	(PhD, 2008; Samsung, Korea)
2001-2004	Jane Owens	(PhD, 2004; Asst Prof, Central College, IA)
2001-2007	Joshua Coe	(PhD, 2007; Staff Scientist, Los Alamos National Lab)
2000-2007	James Hemp	(PhD, 2007; Instructor, University of Utah School of Medicine)
1997-2003	Seth Olsen	(PhD, 2004; Deceased)
1997-2002	Jason Quenneville	(PhD, 2003; Senior Scientist, Spectral Sciences, MA)
1997-1999	Matthew Wander	(MS, 1999; Stony Brook, PhD 2007)
1997-1999	Dana Moore	(MS, 1999; Information Analyst, Cytec Industries, NJ)

**PUBLIC AND PROFESSIONAL SERVICE SINCE 2004**

Sloan Foundation Research Fellowships Program Selection Committee	2019-present
Ford Foundation Fellowships Program Selection Committee	2019
Co-Editor, Annual Reviews in Physical Chemistry (with Mark Johnson)	2011-present
Guest Editor, Comp. in Sci. Eng. Special Issue on "High Performance Computing with Accelerators"	2011
Member, DOE Council on Chemical and Biochemical Sciences	2010-2015

Participant, DOE BES/ASCR Workshop on “Discovery in Basic Energy Sciences: The Role of Computing at the Extreme Scale,” Washington, DC	2009
Chair, ACS Theoretical Chemistry Subdivision	2008
Associate Editor, Journal of Chemical Physics	2007-present
Editorial Board, Advances in Chemical Physics	2007-2009
Guest Editor, Chemical Physics Special Issue on “Ultrafast photoinduced processes” in honor of W. Domcke	2007
Guest Editor, J. Phys. Chem. Festschrift in Honor of J. T. Hynes	2007
Chair-Elect, ACS Theoretical Chemistry Subdivision	2007
Advisory Board, Physical Chemistry Chemical Physics	2006-2011
Advisory Editor, Journal of Physical Chemistry	2006-2010
Advisory Board, Chemical Physics	2006-2009
Vice-Chair, ACS Theoretical Chemistry Subdivision	2006
Advisory Editor, Theoretical Chemistry Accounts	2005-2010
Research Associateship Program Selection Committee, National Research Council	2005-2008
Editorial Board Member, Journal of Chemical Physics	2005-2007
NIH Pioneer Award Selection Committee	2006-2008
ACS Award Selection Committee	2004-2007
Steering Committee, NSF Workshop on Cyber-Enabled Chemistry	2004
NSF-CHE Committee of Visitors	2000, 2004
Participant, NSF Workshop on CyberScience/Cyberinfrastructure	2004
Site visitor, panel reviewer, and <i>ad hoc</i> reviewer for various federal agencies	1996-present
<i>Ad hoc</i> reviewer for various journals	1996-present

#### UNIVERSITY, CAMPUS, AND DEPARTMENTAL SERVICE (Stanford and SLAC only)

Committee on Undergraduate Standards and Policies	2019-2020
School of Humanities and Sciences Dean Search Committee	2017-2018
SLAC Faculty Retreat organizing committee	2016
Alliance for Graduate Education and the Professoriate (AGEP), Co-PI	2014-2018
Enhancing Diversity in Graduate Education (EDGE), Faculty Mentor	2013-present
Raising Interest in Science and Engineering (RISE), Faculty Mentor	2012-present
Chair, LCLS SLAC/Stanford search committee	2012-2014
Academic Computing and Information Services (C-ACIS) Committee	2012-2014
Co-chair (w/ V. Pande), Stanford Research Computing Facility Committee	2010-2012
Stanford and SLAC faculty search committees	2010-present
Chemistry Department service committees	2010-present
Diversity Liaison, Chemistry	2009-present
Chair, SLAC Midrange Computing Committee	2009
SLAC CIO Search Committee	2009

#### CONFERENCES CHAIRED AND ORGANIZED

Chair, American Conference of Theoretical Chemistry	2020
Organizer (w/S. Kais), ACS Symposium on Information Theory and Dynamics in honor of Raphael Levine, Boston, MA	2018
Vice-Chair, American Conference of Theoretical Chemistry	2017
Organizer (w/A. Trefethen), EPSRC/NSF Workshop on Software Development for Grand Challenges in the Chemical Sciences, Oxford, UK	2011

Organizer (w/V. Kindratenko, T. Dunning, R. J. Harrison and J. Madura), ACS Symposium on Chemical Computations on General Purpose Graphics Processing Units, Boston, MA	2010
Chair, Gordon Research Conference on Atomic and Molecular Interactions, Colby-Sawyer College, New London, NH	2010
Organizer (w/G. Scuseria), DOE Workshop on Theories of Excited States in Molecules and Nanostructures, Baltimore, MD	2010
Session chair and discussion leader, CECAM Workshop on Computational, Theoretical and Experimental Challenges to Exploring Coherent Quantum Dynamics in Many-Body Systems, Dublin, Ireland	2010
Organizer (w/V. Kindratenko, W. Hwu, R. Wilhelmson, and R. Brunner), Path to Petascale: Adapting GEO/CHEM/ASTRO Applications for Accelerators and Accelerator Clusters, Urbana, IL	2009
Vice-chair, Gordon Research Conference on Atomic and Molecular Interactions, Colby-Sawyer College, New London, NH	2008
Session Chair, American Conference on Theoretical Chemistry, Evanston, IL	2008
Organizer (w/S. Matsika), ACS Symposium on Excited Electronic States in Chemistry and Biology: Theory and Experiment, Boston, MA	2008
Organizer (w/A. Stolow), APS Focus Session on Nonadiabatic Molecular Dynamics and Control at Conical Intersections, Denver, CO	2007
Organizer (w/D. Ceperley, D. Johnson, and R. Martin), Summer School on <i>Ab Initio Molecular Dynamics Simulation Methods in Chemistry</i> , Urbana, IL	2006
Organizer (w/J. Saltiel and others), NSF Workshop on Photochemistry, Salvador, Brazil	2006
Organizer (w/E. DeSturler and D. Johnson), SIAM Minisymposium on <i>Multiscale Modeling from Materials to Biology</i> , Orlando, FL	2005
Session Chair, ACS Symposium on <i>Quantum/Classical Calculations in Chemistry and Biophysics</i> , Philadelphia, PA	2004
Session Chair, Conference on Excited State Processes in Electronic and BioNanoMaterials, Los Alamos, NM	2003
Organizer (w/ Roberto Car), ACS Symposium on First Principles Simulation of Chemical Dynamics, Chicago, IL	2001
Organizer (w/ D. Ceperley, D. Johnson, R. Martin, and E. deSturler), Summer School on Computational Materials Science, Urbana, IL	2001
Session Chair, W. H. Miller 60th Birthday Symposium, San Francisco, CA	2001
Organizer and Session Chair, Midwest Theoretical Chemistry Conference, Urbana, IL	2001
Session Chair, ACS Symposium on Dynamics in Molecular Systems, Las Vegas, NV	1997

## INVITED LECTURES SINCE 2001

### DISTINGUISHED ADDRESSES

Condon Lecturer, University of Colorado at Boulder	2019
Stanford in Mexico Lecturer, Mexico City, Mexico	2018
McElvain Lecturer, University of Wisconsin at Madison	2018
Student-Selected Speaker, University of Illinois at Urbana Champaign	2018
Plenary Lecturer, World Association of Theoretical Chemists, Munich	2017
Plenary Lecturer, Iberian Joint Meeting on Atomic and Molecular Physics, Barcelona	2017
Frontiers in Chemical Research Lecturer (Series of 3 lectures), Texas A&M	2017
Kahn Lecturer, University of New Mexico	2017
J. C. Bose Endowment Lecturer, Kolkata, India	2017

Keynote Lecturer, Computational Chemistry GRC, Girona, Spain	2016
Kroto Lecturer, Florida State University	2016
Keynote Lecturer, IUPAC-2015, Busan, South Korea	2015
Mulliken Lecturer, University of Georgia	2014
Inaugural Isaiah Shavitt Lecturer, Technion, Israel (Series of 4 lectures)	2014
Student-Selected Speaker, Princeton University (Student-Selected Speaker)	2014
MPS Distinguished Lecturer, National Science Foundation	2014
Xingda Lecturer, Peking University, China	2014
Plenary Lecturer, 22 <sup>nd</sup> International Conference on Physical Organic Chemistry (ICPOC-22), Ottawa, Canada	2014
Gunning Lecturer, University of Alberta (Series of 3 Lectures)	2013
Albrecht Lecturer, Cornell University	2013
Distinguished Physical Chemistry Lecturer, University of Nevada, Reno (Series of 2 lectures)	2013
Closs Lecturer, University of Chicago	2011
Jeremy A. Musher Lecturer, Hebrew University, Jerusalem (Series of 2 lectures)	2011
Charles A. McDowell Lecturer, University of British Columbia	2010
Plenary Lecturer, DPG Spring Meeting, Dresden	2010
Western Switzerland 3 <sup>eme</sup> Cycle Lecturer (Series of 5 lectures)	2010
Plenary Lecture, MQM2010, Berkeley, CA	2010
Alumni of Merit, Carol Morgan School, Santo Domingo, Dominican Republic	2008
Woodward Lecturer, Harvard University	2006
William Thomas Jackson Lecturer, Eureka College	2006

**DEPARTMENTAL SEMINARS**

University of California at Davis	2018
New York University	2017
University of Texas at San Antonio	2017
University of Bristol	2017
ETH Zurich	2017
California Institute of Technology	2016
University of Connecticut, Physics Colloquium	2016
Michigan State University	2016
Stockholm University, Stockholm, Sweden	2016
Uppsala University, Uppsala, Sweden	2015
Stockholm University, Stockholm, Sweden	2015
Linkoping University, Linkoping, Sweden	2015
Kyoto University	2015
University of Calgary	2015
Marmara University, Istanbul, Turkey	2015
Northwestern University	2014
MIT/Harvard/Boston University Theoretical Chemistry Series	2014
University of Colorado at Boulder	2012
California Institute of Technology	2012
Simon Fraser University, Vancouver, Canada	2011
University of British Columbia, Vancouver, Canada	2011
University of Victoria, Victoria, Canada	2011
Queen's University, Kingston, Ontario, Canada	2010



University of California at San Diego	2010
Duke University	2010
Frontiers in Chemical Physics and Analysis Seminar, PNNL	2009
University of California at Davis, Biophysics Program	2009
University of Washington at Seattle	2009
Harvard University, Initiative for Innovative Computing	2009
Virginia Tech University	2009
Yale University	2009
University of Pittsburgh	2008
University of California at Irvine	2008
Stanford University	2007
Ohio State University	2007
Massachusetts Institute of Technology	2007
University of California at Berkeley	2007
University of Wisconsin at Madison	2007
Indiana University	2006
California Institute of Technology (Series of 2 lectures)	2006
Ecole Normale Supérieure, Paris	2006
Argonne National Laboratories	2006
University of California at Los Angeles	2005
Emory University	2005
Cornell University, Baker Symposium, "Frontiers in Theoretical Chemistry"	2005
Temple University	2005
Wayne State University	2004
University of California at Irvine	2004
University of Puerto Rico at Rio Piedras	2004
Northwestern University	2003
Iowa State University	2003
Indiana State University	2003
Stearns Institute for Molecular Sciences, Ottawa, Canada (Series of 2 lectures)	2003
Calvin College	2003
Princeton University (Series of 4 lectures)	2003
Rutgers University	2003
Pennsylvania State University	2003
University of Colorado at Boulder	2002
Johns Hopkins University	2002
Texas Tech University	2002
University of Texas at Austin	2002
University of Chicago	2001
Rice University	2001
University of California at San Diego	2001
University of Nevada at Reno	2001
University of California at Davis	2001
University of California at Berkeley	2001
Stanford University	2001
Emory University	2001
University of Georgia	2001
Georgia Institute of Technology	2001

Massachusetts Institute of Technology	2001
MIT/Harvard/Boston University Theoretical Chemistry Series	2001
University of California at Santa Barbara	2001
University of Southern California	2001
University of California at Los Angeles	2001
California Institute of Technology	2001
Wabash College	2001
University of Pennsylvania	2001

## MEETINGS AND WORKSHOPS

International Symposium on Quantum Effects in Chemistry and Biology, Shanghai, China	2019
ACS Symposium on "Sustainable Software for Computational Molecular Science," Orlando, FL	2019
10th International Meeting on Photodynamics and Related Aspects, Cartagena, Colombia	2018
Photoinduced Processes in Embedded Systems, Pisa, Italy	2018
Grand Challenges in the Chemical Sciences, Israel Academy of Sciences, Jerusalem, Israel	2018
CECAM Workshop on "Nonadiabatic Dynamics in Three Flavors," Lausanne, Switzerland	2018
58th Sanibel Meeting, St. Simons Island, GA	2018
NCCR Molecular Ultrafast Science and Technology (2x 90 min lectures), Grindelwald, Switzerland	2018
CHAMPS: Chemistry and Mathematics in Phase Space, Bristol, UK	2018
American Conference on Theoretical Chemistry, Boston, MA	2017
Workshop on "Quantum Effects in Condensed Phase Systems," Telluride, CO	2017
Computational Materials Science, Warwick, UK	2017
Recent Advances in Many-Electron Theory, Goa, India	2017
GAMESS7557 Symposium, Kauai, HI	2017
10th MACCCR Fuel and Combustion Research Review, Chicago, IL	2016
Theory and Applications of Computational Chemistry (TACC), Seattle, WA	2016
Penn Conference on Theoretical Chemistry, Philadelphia, PA	2016
Workshop on Dynamical Quantum Effects in Molecular Processes, New York, NY	2016
9th International Meeting on Photodynamics and Related Aspects, Mendoza, Argentina	2016
Shanghai International Symposium on Computational Chemistry, Shanghai, China	2015
1st Mueunjae Symposium on Chemistry and Light, POSTECH, Korea	2015
Workshop on "Excited States: Electronic Structure Theory and Dynamics," Telluride, CO	2015
Workshop on "Quantum Effects in Condensed Phase Systems," Telluride, CO	2015
ACS Symposium on "Design Principles of Functional Macromolecular Materials," Denver, CO	2015
ACS Symposium on "Modeling Excited States of Complex Systems," Denver, CO	2015
ICQC Satellite Symposium on "Novel Computational Methods for Quantitative Electronic Structure Calculations," Kobe, Japan	2015
Dynamic of Molecular Collisions XXV, Asilomar, CA	2015
XL Congreso de Quimicos Teoricos de Expresion Latina, San Cristobal, Ecuador	2014
50th Symposium on Theoretical Chemistry, Vienna, Austria	2014
American Conference on Theoretical Chemistry (ACTC), Telluride, CO	2014
DAMOP Invited Session on "Non-Born-Oppenheimer Dynamics," Madison, WI	2014
LCLS/SSRL Workshop on "Characterizing and Controlling Chemical Dynamics," Menlo Park, CA	2014
LLNL Computational Chemistry and Materials Science Summer Institute	2014

Workshop on “Condensed Phase Dynamics,” Telluride, CO	2014
ACS Symposium on “Quantum Mechanics in Many Dimensions,” Indianapolis, IN	2013
ACS Symposium on “Frontiers in Reaction Dynamics,” New Orleans, LA	2013
Third International Symposium on Computational Sciences, ISCS Shanghai, China	2013
SUNCAT Summer School, Menlo Park, CA	2013
Workshop on “Quantum Effects in Condensed Phase Systems,” Telluride, CO	2013
CECAM Workshop on “Many-dimensional quantum dynamics with (non) classical trajectories,” Lausanne, Switzerland	2013
Ultrafast X-Ray Summer School (UXSS), Hamburg, Germany	2013
Mathematical Methods in Quantum Molecular Dynamics, Banff, Canada	2013
CECAM Workshop on “High-Dimensional Quantum Dynamics,” Birmingham, UK	2013
GRC on Atomic and Molecular Interactions, Easton, MA	2012
157 <sup>th</sup> Faraday Discussion on Molecular Reaction Dynamics in Gases, Liquids and Interfaces, Assisi, Italy	2012
SimTech-CECAM Workshop on “Advanced Methods and Applications in Quantum Chemistry,” Stuttgart, Germany	2012
Quantum Molecular Dynamics (Millerfest), Berkeley, CA	2012
CUSO Summer School “From Electronic Structure to Quantum Dynamics,” Villars, Switzerland (Series of 3 lectures)	2012
APS Focus Session on “GPUs in Computational Physics,” Dallas, TX	2011
XXXVII Congreso de Quimicos Teorico de Expresion Latina, Riviera Maya, Mexico	2011
XVI Simposio Brasileiro de Quimica Teorica, Ouro Preto, Brazil	2011
ISTCP-VII, Tokyo, Japan	2011
EXCST2011, “Excited States and non-adiabatic processes in complex systems,” St. Feliu de Guixols, Spain	2011
WATOC, Santiago de Compostela, Spain	2011
2 <sup>nd</sup> IQTCUB Symposium, Barcelona, Spain	2011
ACS PacifiChem Symposium, “Frontiers in State-to-State Dynamics,” and “Challenges and Solutions to Accurate Calculations on Large Molecular Systems and Condensed Phases,” Honolulu, HI	2010
KITP Program on “X-Ray Frontiers”	2010
ACS Symposium on “Challenges in DFT,” Boston, MA	2010
GRC on Electron Donor-Acceptor Interactions, Salve Regina, RI	2010
CECAM Workshop on “Adiabatic and Non-Adiabatic Methods in Quantum Dynamics,” EPFL, Switzerland	2010
GRC on Computational Chemistry, Les Diablerets, Switzerland	2010
European Computational Chemistry Conference, Lund, Sweden	2010
Summer School on Theoretical Chemistry (5 lectures), Beijing, China	2010
Canadian Society of Chemistry, Symposium on “Coherence and Decoherence in Molecular Dynamics,” Toronto, CA	2010
CECAM Workshop on Computational, Theoretical and Experimental Challenges to Exploring Coherent Quantum Dynamics in Many-Body Systems, Dublin, Ireland	2010
International Workshop on Science with Free Electron Lasers	2010
Mariapfarr Winter School on Dynamics in Excited States, Mariapfarr, Austria	2010
Wavepackets, Chaos and Scattering: From Chemistry to Physics and Back, ITAMP, Harvard University, MA	2010
Symposium on Applications of Graphics Processing Units in Chemistry and Materials Science, University of Pittsburgh, PA	2010

Gordon Conference "Photoions, Photoionization and Photodetachment," Galveston, TX	2010
MRS Symposium, Boston, MA, "Mechanochemistry in Polymers"	2009
2 <sup>nd</sup> International Conference on Self-Healing Materials, Chicago, IL	2009
ACS Symposium, Salt Lake City, UT, "Advances in Electronic Structure Theory and First Principles Dynamics"	2009
45 <sup>th</sup> Symposium on Theoretical Chemistry, Dusseldorf, Germany	2009
CREST International Symposium on Theory and Simulations of Complex Molecular Systems, Kyoto, Japan	2009
DOE Workshop on The Future of Ultrafast Soft X-Ray Science, LBNL, CA	2009
Gordon Conference "TDDFT," New London, NH	2009
ACS Symposium, Philadelphia, PA, "Spectroscopic Probes of Chemical Dynamics in Gaseous and Condensed Phases"	2008
ACS Symposium, New Orleans, LA, "Optical Probes of Dynamics in Complex Environments"	2008
WATOC 2008, Sydney, Australia	2008
Symposium in honor of Wolfgang Domcke, Garching, Germany	2008
Workshop on "Computational Biophysics with Chemical Accuracy," Antigua	2008
CCP6 Workshop on "Multidimensional Quantum Mechanics with Trajectories," Leeds, England	2008
ACS Symposium, Boston, MA, "Bold Predictions in Theoretical Chemistry"	2007
ACS Symposium, Chicago, IL, "Computers in Chemistry and Pharmaceutical Research" and "Capturing Complexity in Physical Sciences Simulation"	2007
47 <sup>th</sup> Sanibel Symposium, St. Simons Island, GA	2007
ICCMSE Symposium in honor of Yngve Ohrn, Corfu, Greece	2007
Institute Of Physics Workshop on Nonadiabatic Molecular Dynamics, London, England	2007
CECAM Workshop on Condensed Phase Quantum Dynamics, Dublin, Ireland	2007
Femtochemistry VIII, Oxford, England	2007
Gordon Conference "Photochemistry," Smithfield, RI	2007
APS Focus Session, Baltimore, MD, "Frontiers in Computational Chemical Physics"	2006
Gordon Conference, "Electronic Spectroscopy," Les Diablerets, Switzerland	2006
6 <sup>th</sup> Canadian Computational Chemistry Conference, Vancouver, Canada	2006
XIIth International Congress of Quantum Chemistry, Kyoto, Japan	2006
Gordon Conference "Atomic and Molecular Interactions," New London, NH	2006
Workshop on Real Time and Interactive Digital Media Supercomputing, Austin, TX (in conjunction with 12 <sup>th</sup> International Symposium on High Performance Computer Architecture)	2006
ACS PacifiChem Symposium, Honolulu, HI, "Photophysical Dynamics in Biological Molecules" and "Photoisomerization Processes: Torsional Relaxation and Hula-twist"	2005
American Conference on Theoretical Chemistry, Los Angeles, CA	2005
Dynamics of Molecular Collisions, Asilomar, CA	2005
SIAM Symposium, Orlando, FL, "Multi-Scale Methods From Materials to Biology"	2005
CECAM Workshop on Ab Initio Molecular Dynamics Beyond Density Functional Theory, Lyon, France	2005
Workshop on Classical and Quantum Dynamical Simulations in Chemical and Biological Physics, Dresden, Germany	2005
Excited State Processes in Electronic and Bio-Materials Workshop, Center for Nonlinear Studies, Los Alamos, NM	2005

ACS Symposium, Philadelphia, PA, “Quantum/Classical Calculations in Chemistry and Biophysics”	2004
ACS Symposium, Anaheim, CA, “Mixed Quantum, Classical and Semiclassical Dynamics”	2004
APS Focus Session, Montreal, Canada, “Structure and Dynamics of Proteins”	2004
CECAM Workshop on Development of Methods for Quantum Dynamics in the Condensed Phase, Lyon, France	2004
127 <sup>th</sup> Faraday Discussion on Nonadiabatic Effects in Chemical Dynamics, Oxford, England	2004
3 <sup>rd</sup> International Meeting on Photodynamics, Havana, Cuba	2004
Plenary Lecture, 36 <sup>th</sup> Midwest Theoretical Chemistry Conference, Lansing, MI	2004
7 <sup>th</sup> Symposium on Molecular Reaction Dynamics in Condensed Matter, Laguna Beach, CA	2004
ACS Symposium, New Orleans, LA, “Recent Developments and Applications of Time-Dependent DFT and Related Ab Initio and Semiempirical Methods” and “New Electronic Structure Methods: From Molecules to Materials”	2003
Sanibel Symposium, St. Augustine, FL	2003
Femtochemistry VI, Paris, France	2003
Symposium on Multidimensional Quantum Reaction Dynamics, Berlin, Germany	2003
APS Symposium, Indianapolis, IN, “Protein Dynamics: Photoinduced Dynamics”	2002
Workshop on Quantum Dynamics in Condensed Phase Systems, Crete, Greece	2002
Workshop on Quantum Dynamical Concepts: From Diatomics to Biomolecules, Dresden, Germany	2002
CECAM Workshop on Methods for Computer Simulation of Non-adiabatic Charge Transfer Processes in Condensed Phases, Lyon, France	2002
2 <sup>nd</sup> International Workshop on Photodynamics from Isolated Molecules to Condensed Phases, Havana, Cuba	2002
Workshop on Ab Initio Direct Dynamics, Maui, HI	2002
Beckman Young Investigators Symposium, Irvine, CA	2002
Beckman Scholars Symposium, Irvine, CA	2002
Gordon Conference “Atomic and Molecular Interactions,” Bristol, RI	2002
Frontiers of Theoretical Chemistry, Tokyo, Japan	2001
34 <sup>th</sup> Midwest Theoretical Chemistry Conference, Minneapolis, MN	2001
Excited State Processes in Electronic and Bio-Materials Workshop, Center for Nonlinear Studies, Los Alamos, NM	2001
XVIII Conference on Dynamics of Molecular Collisions, Copper Mountain, CO	2001
Gordon Conference “Biological Molecules in the Gas Phase,” New London, CT	2001
13 <sup>th</sup> Annual Workshop on Recent Developments in Electronic Structure Theory, Princeton, NJ	2001

## PROFESSIONAL SOCIETY MEMBERSHIPS

American Chemical Society  
 American Physical Society  
 American Association for the Advancement of Science  
 Biophysical Society

## PEER-REVIEWED PUBLICATIONS

247. *Quantum Computation of Electronic Transitions Using a Variational Quantum Eigensolver*, R. M. Parrish, E. G. Hohenstein, P. L. McMahan, and T. J. Martínez, *Phys. Rev. Lett.*, **122**, 230401 (2019). DOI: doi.org/10.1103/PhysRevLett.122.230401

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