

## DONALD G. TRUHLAR

### Personal and contact information

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### Education

St. Mary's College of Minnesota, B. A., Chemistry, summa cum laude, 1965.

California Institute of Technology, Ph. D., Chemistry, 1970.

Graduate adviser: Aron Kuppermann (1917-2011)

### Appointments

University of Minnesota:

Department of Chemistry

Member of Graduate Faculty, 1969-present

Assistant Professor, 1969-72

Associate Professor, 1972-76

Professor, 1976-2006

Director of Graduate Studies, 1986-88

George Taylor Institute of Technology Professor, 1993-1998

Institute of Technology Distinguished Professor, 1998-2001

Lloyd H. Reyerson Professor, 2002-2006

Regents Professor, 2006-present

Chemical Physics Program

Member of Graduate Faculty, 1969-present

Head and Director of Graduate Studies, 1980-84, 1992-95, 1998-99

Supercomputing Institute

Fellow, 1985-present

Acting Scientific Director, 1987-88

Director, 1988-2006

Graduate Program in Scientific Computation

Founding Director of Graduate Studies, 1990-96, 2002

Charter Member of Graduate Faculty, 1990-2018

Graduate Minor Program in Nanoparticle Science and Engineering

Charter Member of Graduate Faculty, 2002-2015

Chemical Theory Center, Department of Chemistry

Founding director, 2005-2011; member, 2005-present

Nanoporous Materials Genome Center

Deputy director, 2018-2022

Battelle Memorial Institute: Columbus, Ohio, Visiting Fellow, 1973 (host: Isaiah Shavitt).

Joint Institute for Laboratory Astrophysics, Boulder, Colorado: Visiting Fellow, 1975-76  
(host: William Reinhardt).

## **Academies**

American Academy of Arts and Sciences, 2015-  
International Academy of Quantum Molecular Science, 2006-  
National Academy of Sciences USA, 2009-

## **Fellow, Societies and Associations**

American Association for the Advancement of Science (AAAS), Fellow since 1994  
American Chemical Society (ACS), Fellow since 2009 (inaugural year of fellows program)  
American Physical Society (APS), Fellow since 1986  
Chemical Research Society of India (CRSI), Honorary Fellow since 2019  
Chinese Chemical Society (CCS), Honorary Fellow since 2015  
Royal Society of Chemistry (RSC), Fellow since 2009  
World Association of Theoretical and Computational Chemists (WATOC), Fellow since 2006

## **Major Awards and Honors, Extramural**

Alfred P. Sloan Foundation Research Fellowship, 1973  
Fellow of the American Physical Society, 1986  
“for his many outstanding contributions to theoretical chemical dynamics and our understanding of chemical reactions”  
NSF Creativity Award, 1993  
“scattering theory and calculations for chemical reactions and molecular energy transfer”  
Fellow of the American Association for the Advancement of Science, 1994  
“honored for advances in quantum mechanical scattering theory and theoretical kinetics and for applying supercomputational methods to chemical dynamics, energy transfer, potential energy surfaces, and path integrals”  
American Chemical Society Award for Computers in Chemical and Pharmaceutical Research, 2000  
“for his pioneering work combining theoretical chemistry and digital computation to further our fundamental understanding of chemical reactivity and molecular interactions through visionary accomplishments in the areas of potential energy functions, accurate quantum dynamics, variational transition state theory, and the use of electronic structure theory for calculations of reaction rates and solvation effects”  
Minnesota Award (ACS Minnesota Section), 2003  
“outstanding contributions to the chemical sciences”  
National Academy of Sciences Award for Scientific Reviewing, 2004  
“for his incisive reviews on transition-state theory, potential energy surfaces, quantum scattering theory, and solvation models, which have informed and enlightened the chemical physics community for a generation”  
American Chemical Society Peter Debye Award for Physical Chemistry, 2006

“for fundamental contributions to the theory of chemical reaction dynamics, especially quantum mechanical scattering theory and variational transition state theory”

Lise Meitner Lectureship Award for the year 2006

for “computational quantum chemistry as a research tool in chemistry, through his numerous contributions to the generation of practical methods for electronic structure, potential energy surfaces, solvent models, reaction rates, and dynamics.”

Donald G. Truhlar Festschrift, 2006

*Journal of Physical Chemistry A*, Volume 100, Number 2 (January 19, 2006)

Schrödinger Medal of The World Association of Theoretical and Computational Chemists (WATOC), 2006

“for his outstanding contributions to the theory and computation of chemical reaction dynamics in ground and excited states.”

Fellow of the World Association of Theoretical and Computational Chemists, 2006

See <http://www.ch.ic.ac.uk/watoc/>

Dudley Herschbach Prize for Molecular Collision Dynamics, 2009

The award, established in 2007 and given every two years at the Conference on the Dynamics of Molecular Collisions, recognizes "excellence in research in collision dynamics...bold and architectural works inspiring and empowering in the field of the dynamics of molecular collisions."

Named a Fellow of the Royal Society of Chemistry (U.K.), 2009

The award was given for outstanding contribution to the chemical sciences. Fellows are entitled to use the designatory letters FRSC after their name.

Elected to Fellowship in the American Chemical Society, 2009

Inaugural year of ACS Fellows Program.

Doctor honoris causa of Technical University of Lodz, Poland, 2010

“for his contributions to the development of quantum chemistry and vivid collaboration with our and other Polish universities”

Distinguished Alumnus Award, St. Mary’s University of Minnesota, 2011

“In recognition as a world-renowned physical chemist who has advanced and transformed chemistry and chemical physics as a distinguished professor, author, and researcher”

Royal Society of Chemistry Chemical Dynamics Award, 2012

“for your many fundamental contributions to the modeling and understanding of chemical reaction dynamics”

International Symposium on Organic Reaction Mechanism: A celebration in honor of Bob Grubbs, Ken Houk, Paul Schleyer, and Don Truhlar

“four of the great chemists of our time,” Peking University, Shenzhen Graduate School, May 8-9, 2013

ACS Physical Chemistry Division Symposium in Honor of Donald G. Truhlar, 2015

“Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular, and Condensed-Phase Systems: A Symposium in Honor of Donald G. Truhlar,” 249th ACS National Meeting, March 22-26, 2015, Denver

Outstanding Referee, American Physical Society, 2015

The Outstanding Referee program of the APS (publisher of the *Physical Review* and *Physical Review Letters*), recognizes a "small percentage" of "outstanding referees" whose "reports have helped us to advance and diffuse the knowledge of physics, while creating a resource that is invaluable to authors, researchers, students and readers." Like Fellowship in the APS, this is a lifetime award.

Elected as Honorary Fellow of the Chinese Chemical Society, 2015

“Honorary Fellow is the highest honor that CCS bestows on an individual and it is only conferred to the distinguished chemists of the world who have made significant contributions to the advancement of chemistry as well as to the development of Chinese Chemistry and the Society. The total number is limited to 100 individuals worldwide.” At the time of the award, there were 34 previous awardees.

American Physical Society 2016 Earle K. Plyler Prize for Molecular Spectroscopy and Dynamics

“For extraordinarily broad and seminal advances in chemical kinetics, dynamics, and spectroscopy through pioneering and incisive work in the development and application of variational transition state theory, electronic structure calculations, and quantum mechanical scattering methods.”

Honorary Professor of the Dalian Institute of Chemical Physics

Chinese Academy of Sciences, awarded June 8, 2017

American Chemical Society Award in Theoretical Chemistry, 2019

To recognize innovative research in theoretical chemistry that either advances theoretical methodology or contributes to new discoveries about chemical systems. The citation reads, “For creative contributions to theoretical chemistry, in electronic structure, chemical dynamics, continuum solvation, and the development of new density functionals for practical calculations of thermochemical quantities.”

Elected as Honorary Fellow of the Chemical Research Society of India (CRSI), 2019

According to the CRSI, “Honorary Fellowship is conferred on eminent chemists in recognition of their monumental contributions to chemistry and related areas.” A total of 57 chemists (16 from the USA) were elected to Honorary Fellowship in the years 2000-2018.

Virtual Issue of *Journal of Chemical Theory and Computation*, 2020

“Honoring Donald G. Truhlar's Contributions: This Special Issue recognizes the contributions to *JCTC* of Prof. Truhlar and his group at the University of Minnesota.” First person to receive this honor.

<https://pubs.acs.org/page/jctcce/vi/truhlar.html>

Honorary Editor, *Theoretical Chemistry Accounts*, 2021

Second person to receive this honor. The first was Klaus Ruedenberg.

**Selected Awards and Honors, University of Minnesota**

Elected Fellow of Minnesota Supercomputing Institute, 1985

George Taylor/Institute of Technology Alumni Society Distinguished Service Award, 1998

“for his extramural leadership in internationally recognized chemistry journals and his intramural development of the Supercomputing Institute”

Inventor Recognition Award, 2005

Regents Professor, University of Minnesota, 2006

“The Regents Professorship is the University's highest recognition for faculty excellence. The award honors faculty whose especially distinguished accomplishments in teaching and scholarship or creative work have contributed uniquely to the University and to the public good.”

University Innovations Award, 2011

“in appreciation of your commitment to research and innovation at the University”

Outstanding Adviser Award of the Graduate and Professional Student Assembly 2013

"to recognize faculty members who are exemplary in their role as a mentor and adviser"

2015 Council of Graduate Students Outstanding Faculty Award

“to recognize contributions of faculty members who go above and beyond in their work with graduate students.”

2016 Outstanding Advising and Mentoring Award

April 2016. Recognized by the Council of Graduate Students and Student Conflict Resolution Center. Seven awards university-wide.

2020 Award for Outstanding Contributions to Graduate and Professional Education

This award was established “to recognize contributions to post baccalaureate, graduate, and professional education. Recipients are chosen for excellence in instruction; involvement in students' research, scholarship, and professional development; development of instructional programs; and advising and mentoring of students.”

Membership in the Academy of Distinguished Teachers

The title "Distinguished University Teaching Professor" is conferred upon members. Conferred Feb. 2020.

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**RESEARCH**

Google Scholar link: <https://scholar.google.com/citations?user=1gaf87YAAAAJ&hl=en>

*Major contribution areas:*

Variational transition state theory  
 Semiclassical tunneling methods  
 Converged quantum dynamics for chemical kinetics, scattering, and resonances  
 Quantum mechanical and semiclassical methods for photochemical dynamics  
 Universal solvation models, including SMD  
 Vibrational anharmonicity  
 Minnesota functionals for Kohn-Sham density functional theory  
 Multi-configuration pair-density functional theory

*More detailed summary:*

Professor Truhlar's research is in theoretical and computational chemical physics and physical chemistry, with emphases on quantum mechanics, dynamics, kinetics, solvation, electronic structure, and thermochemistry. Special areas of focus are:

- electronic structure theory: wave function theory, density functional theory, and combined quantum mechanical–molecular mechanical methods
- the development of broadly accurate density functionals and density functional methods for electronic structure calculations by Kohn-Sham theory and multiconfiguration pair-density functional theory
- computational thermochemistry, including free energies of complex species in the gas phase and solution, solvation free energies, electrochemistry, and nanothermodynamics
- the study of photoactivated processes, for which his work includes excitation energies, potential energy surfaces and their couplings, and multi-state dynamics
- accurate quantum mechanical scattering theory for electron scattering, energy transfer, chemical reactions, and electronically nonadiabatic processes
- incorporation of quantum effects in semiclassical dynamics, including tunneling, vibrational quantization, coherence and decoherence, and electronic state switching
- variational transition state theory applied to gas-phase and condensed-phase reactions, with special emphasis on atmospheric chemistry, combustion, enzyme kinetics, nanodusty plasmas, and surface science
- quantum mechanical treatment of vibrations, including multistructural effects and torsions
- transition metal chemistry for catalysis and magnetic properties
- metal–organic frameworks, especially for catalysis
- new methods for path integral calculations in quantum mechanical statistical mechanics
- battery development: structure, electromotive force, capacity, and transport

## Bibliography

1329 journal articles, 89 book chapters, 14 books edited.

Bibliography: <http://truhlar.chem.umn.edu/publications>

## Citation Statistics

Statistics from Google Scholar, Oct. 5, 2022:

Number of citations: 206,653. h-index: 189. i10 index: 1328.

22 articles with 1000 or more citations.

<https://scholar.google.com/citations?user=1gaf87YAAAAJ&hl=en>

Statistics from Clarivate Web of Science, Oct. 5, 2022:

Number of citations: 164,896 in 79,177 articles. h-index: 169.

*Chemistry World* h-index ranking of living chemists, April 15, 2010: 15th among all chemists worldwide, 3rd among theoretical chemists (behind M. Karplus and R. Hoffmann)

Research.com, May 22, 2022: Out of 35,754 profiles examined for the discipline of Chemistry, Professor Truhlar had a ranking of #14 in the world and #9 in the United States. The only theorists ranked higher were J. Nørskov (Denmark) and M. Karplus (US).

Listed by Thomson Reuters in *The World's Most Influential Scientific Minds*

Listed by Clarivate as *Highly Cited Researcher*

In December 2016, on the 120th anniversary of the founding of the Journal of Physical Chemistry, the article "Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions" (A. V. Marenich, C. J. Cramer, and D. G. Truhlar, 2009) was announced to be the top 25 most highly cited papers in the history of the journal, out of 154,000 papers published, and was the only article published in the most recent 12 years that was included in the announced list of the top 25.

## Research support

### Funding

#### Government:

National Science Foundation

U.S. Department of Energy, Office of Basic Energy Sciences

Air Force Office of Scientific Research

Army Research Office

Office of Naval Research

National Institute of Standards and Technology: Advanced Technology Project  
with Phillips Petroleum

National Institutes of Health

National Aeronautics and Space Administration

Minnesota Dept. of Employment and Economic Development

#### Foundations:

Petroleum Research Fund of the American Chemical Society

Sloan Foundation

#### Industry:

Cray Research, Inc.

Control Data Corporation

Kodak Corporation

University of Minnesota:  
 Department of Chemistry  
 Board of Regents  
 University of Minnesota Graduate School  
 University of Minnesota Institute of Technology  
 Minnesota Supercomputing Institute

Supercomputing grants and extramural computational resource grants:  
 Minnesota Supercomputing Institute  
 National Center for Atmospheric Research  
 National Resource for Computation in Chemistry  
 NSF supercomputer program (Pittsburgh Supercomputer Center, National  
 Aerodynamic Simulation Facility, San Diego Supercomputer Center)  
 Army High-Performance Computing Research Center  
 Maui High Performance Computing Center  
 William R. Wiley Environmental Molecular Sciences Laboratory (including  
 computational grand challenge grants)  
 U.S. Dept. of Energy INCITE awards (Innovative and Novel Computational  
 Impact on Theory and Experiment)  
 National Energy Research Scientific Computing Center

## SYNERGISTIC ACTIVITIES AND SERVICE

Professional society service to ACS and APS:

### ***American Chemical Society:***

Physical Chemistry Division: Executive Committee, 1980-89, Executive Committee  
 Nominating Committee, 1991

*Subdivision of Theoretical Chemistry: Secretary*, 1981-89, Nominating Committee,  
 1994-95

National Councilor, 1985-87 (elected by Phys. Chem. Division),  
 canvassing committees, 1991-93, 1999-2004, chair, 2001-2002

Task Force on Publication in Molecular Modeling, chair, 1992

award committees, including chair, details confidential

symposium organizer, 1980,84,87,90,94,97,98,99,2002,07,12,13

### ***American Physical Society:***

Topical Group on Few-Body Systems and Multiparticle Dynamics: Nominating  
 Committee, 1988, Program Committee, 1989-90;

Division of Computational Physics: Nominating Committee, 2000-02, Fellows  
 Committee, 2005-06;

Physics and Astronomy Classification Scheme, Working Group on Section 82  
 "Physical/Surface Chemistry", 2000;

Division of Chemical Physics: Executive Committee, 2010-2014, program chair, 2012,  
*Chemical Physics Division Chair*, 2012-13 (elected 2009)

symposium organizer, 2016

award committees, details confidential

Organization of conferences and symposia, organizer or co-organizer:

Conf. on the Dynamics of Molecular Collisions, elected 1981, vice chair 1983, chair 1985



American Conf. on Theoretical Chemistry, elected 1981, vice chair 1984, chair 1987  
 In addition to these two conferences: 13 ACS and APS symposia and seventeen other national and international symposia, workshops, or conferences, 1980-2012  
 Institute for Mathematics and its Applications: Year on Chemistry and Mathematics 2008-09, local organizer.

Editorships:

*Journal of the American Chemical Society*, Assoc. Ed., 1984-2016.

*Theoretical Chemistry Accounts* (formerly *Theoretica Chimica Acta*), Ed., 1985-98, Assoc. Ed., 1998-2001, Chief Advisory Ed., 2001-2020, Honorary Editor, 2021-.

*Computer Physics Communications*, Principal Ed., 1986-2015.

Festschrift issues of *Journal of Physical Chemistry*, co-organizer:

Bryce Crawford 1984; Aron Kuppermann 2001; Bruce Garrett, 2015.

Editor or co-editor: fourteen books.

Editor of book series:

*Understanding Chemical Reactivity* series of Kluwer Academic Publishers, Founding Series Editor, 1990-92, Editorial Advisory Board, 1992-2004.

*Topics in Physical Chemistry* series of Oxford University Press, Founding Series Editor, 1992-99.

*Highlights in Theoretical Chemistry* series of Springer, Founding Series Co-editor, 2012-present.

Associate Editor:

*Journal of Chemical Physics* (published by AIP), Assoc. Ed., 1978-80

Editorial Boards:

*Chemical Physics Letters*, Advisory Ed., 1982-present

*Journal of Physical Chemistry* (published by ACS), Advisory Board, 1985-87

*Reports in Molecular Theory*, Ed. Board, 1989-90;

*Computational Science & Engineering* (published by IEEE), Area Ed., 1993-98

*Advances in Chemical Physics*, Ed. Board, 1993-present

*International Journal of Modern Physics C*, Ed. Board, 1994-2005

*International Journal of Quantum Chemistry*, Advisory Ed. Board, 1996-2000

*Computing in Science and Engineering* (published by APS and IEEE), Applications Ed., 1999-2005

*Journal of Computational Methods in Sciences and Engineering*, Ed. Board, 2001

*PhysChemComm* (published by RSC), Advisory Ed. Board, 2001-03

*Open Chemistry*, Ed. Board, 2003-present (was called *Central European Journal of Chemistry* from 2003 to 2014)

*Journal of Chemical Theory and Computation* (published by ACS), Advisory Board, 2004-present

*Chemical Physics*, Advisory Ed. Board, 2005-present

*Molecules*, Section Ed., 2016-present

*Research* | a *Science* partner journal, Associate Ed., 2018-2022; Advisory Ed., 2022-present

## Recent reviewer recognition:

*Chemical Physics Letters* Certificate of Outstanding Contribution in Reviewing

awarded May 2015 in recognition of the contributions made to the quality of the journal

*Journal of Chemical Physics* Top Reviewer, 2016, 2017, 2019

*Clarivate Top reviewers: in Chemistry*, 2018, 2019, *in Cross-field*, 2019

*International Journal of Quantum Chemistry* Reviewer of the Month, July 2020

“honored for his professionalism, compassion, and collaborative spirit supporting the theoretical and computational chemistry community through his volunteer work as referee ... making a significant, positive, and constructive contribution to the peer-review process.”

**Selected other major national and international service**

Brookhaven National Laboratory: Visiting Committee for the Chemistry Department, 1982-85;

Center for Functional Nanomaterials, review panel, 2008-2009

Council for International Exchange of Scholars: Advisory Screening Committee in Chemistry (selection of Fulbright Fellows), 1977-1980, chairman, 1979-80

National Research Council: Committee on Kinetics of Chemical Reactions, member, 1977-80, nominating committee, 1980; Committee on Chemical Sciences Report, contributor, 1983; Panel for Chemical Physics, National Research Council Board on Assessment of National Bureau of Standards Programs, 1986-88

International Union of Pure and Applied Chemistry (IUPAC): Working Party on Guidelines for Publication of Research Results from Empirical Force Field Calculations, Commission on Physical Organic Chemistry, 1997-8

Maui High Performance Computing Center: Advisory Committee for Chemistry, 1995-97

U. S. Dept. of Energy: Roadmap Committee for Strategic Simulation Initiative in Combustion, 1998

Center for Physical and Computational Mathematics and High-Performance Computing, Ames, Iowa: Review Panel, 2002

Computational Center for Molecular Structure and Interactions, Jackson State University: External Advisory Board, 2002

Princeton-Combustion Energy Frontier Research Center-Combustion Institute Summer School: Advisory Committee, 2009-2016

Catalysis Center for Energy Innovation (CCEI): Advisory Board, 2011

**University service**

Numerous departmental, college, and university-wide committees.

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## TEACHING AND RESEARCH SUPERVISION

### Teaching

Graduate courses taught:

- Chemical dynamics
- Chemical reaction dynamics
- Dynamics
- Foundations of quantum chemistry
- Kinetics
- Molecular quantum mechanics
- Quantum mechanics I, II
- Professional conduct of research (including ethics)
- Reaction dynamics
- Statistical mechanics I, II
- Supercomputer research seminar
- Thermodynamics
- Thermodynamics and statistical mechanics
- Computational chemistry (guest lecturer)
- Computational neuroscience (guest lecturer)

Undergraduate courses taught:

- General chemistry (for engineering students)
- General principles of chemistry I, II
- Quantum chemistry
- Statistical mechanics and reaction kinetics
- Topics in physical chemistry

### Research supervision

Number of research students:

- Undergraduate: 89 (67 publications with 47 different undergraduate coauthors)
- Graduate: 64 completed Ph.D. or both Ph. D. and M. S., 12 completed with M. S., 6 currently working toward Ph. D.
- Postdoctoral: 105

### Selected honors to my research group

Extramural honors awarded to postdoctoral associate I supervised:

- 2020 Yinan Shu: American Chemical Society Division of Physical Chemistry's 2020 Young Investigator Award
- 2020 Yinan Shu: Robin Hochstrasser Young Investigators Award
- 2021 Yinan Shu: Wiley Computers in Chemistry Outstanding Postdoc Award for Spring 2021, American Chemical Society Division of Computers in Chemistry

Extramural honors awarded to graduate students I supervised:

- 1982 Rex T. Skodje: Procter and Gamble Award of the Division of Physical Chemistry of the American Chemical Society for the paper "A General Small-Curvature Approximation for Transition State Theory Transmission Coefficients," J. Phys. Chem. **85**, 3019 (1981)

- 1993 David Chatfield: selected as a Finalist for the 1993 American Physical Society Award for Outstanding Doctoral Thesis Research in Atomic, Molecular, and Optical Physics and presented a Finalist lecture at the First Annual AMO Thesis Award Symposium, May 17, 1993
- 2001 Jason Thompson: Midwest Theoretical Chemistry Conference Dirac Award for Outstanding Graduate Research in Theoretical Chemistry
- 2003 Jason Thompson: Chemical Computing Group Excellence Award for National ACS Meeting
- 2006 Casey Kelly: Chemical Computing Group Excellence Award for National ACS Meeting for paper entitled "Calculation of Acid Dissociation Constants by the SM6 Quantum Mechanical Implicit Solvation Model"
- 2015 Junwei (Lucas) Bao: best poster prize at the 15<sup>th</sup> International Congress of Quantum Chemistry
- 2018 Junwei (Lucas) Bao: Graduate Award in Theoretical Chemistry given by the American Chemical Society Physical Chemistry Division

University-wide and college-wide honors awarded to graduate students I supervised:

- 2007 Nathan Schultz: University of Minnesota Graduate School's "Best Dissertation Award, Physical Sciences and Engineering" for his Ph. D. thesis entitled "Computational Nanoscience"
- 2013 Hannah Leverentz: Honorable Mention for Best Dissertation, graduate School, University of Minnesota for her Ph. D. thesis entitled "The Electrostatically Embedded Many-Body Method for the Efficient Computation of Properties of Atmospherically Relevant Nanoparticles"

Departmental honors (since 1992) awarded to graduate students I have supervised:

John Overend Award for Graduate Research in Physical Chemistry

- 1992 Yi-Ping Liu
- 1994 Wei-Ping Hu
- 1999 Michael D. Hack
- 2001 Ahren Jasper
- 2003 Jingzhi Pu and Jason Thompson (co-recipients)
- 2006 Erin Dahlke
- 2010 Bo Wang
- 2011 Hannah Leverentz
- 2016 Shaohong Li
- 2017 Junwei (Lucas) Bao
- 2021 Jiaxin Ning

John Wertz Award for Outstanding Graduate Research in Chemical Physics

- 1993 Stephen Mielke
- 1997 Yao-Yuan Chuang

Beaker and Bunsen Award, Graduate Student Research Symposium

- 2012 Sijie Luo
- 2016 Junwei (Lucas) Bao

University-wide honors awarded to undergraduate student I supervised:

- 2002 Amos Anderson: Thomas DuBrail Undergraduate Research Award, University of Minnesota
- 2003 Amos Anderson: 2003 Peter Auzins Memorial Scholarship and Senior Prize for outstanding achievement in undergraduate research

Recent fellowships awarded to students in my group

- 2011 Bo Wang: Doctoral Dissertation Fellowship
- 2013 Pragma Verma: Phillips 66 Excellence Fellowship
- 2013 Haoyu Yu: Graham N. Gleysteen Excellence Fellowship
- 2014 Pragma Verma: Doctoral Dissertation Fellowship
- 2014 Chad Hoyer: Newman and Lillian Bortnick Excellence Fellowship
- 2014 Shaohong Li: Graham N. Gleysteen Excellence Fellowship
- 2015 Shaohong Li: Frieda Martha Kunze Fellowship
- 2015 Haoyu Yu: Doctoral Dissertation Fellowship
- 2016 Pragma Verma: Richard D. Amelar and Arthur S. Lodge Fellowship for Outstanding Collaborative Research in Materials
- 2016 Chad Hoyer: Doctoral Dissertation Fellowship
- 2016 Shaohong Li: Doctoral Dissertation Fellowship
- 2016 Kelsey Parker: Excellence Fellowship
- 2017 Junwei (Lucas) Bao: Doctoral Dissertation Fellowship
- 2021 Dayou Zhang: Robert and Jill DeMaster - Excellence Fellowship

### Selected overview articles

- "Variational Transition-State Theory," D. G. Truhlar and B. C. Garrett, *Accounts of Chemical Research* **13**, 440-448 (1980).
- "Quantum Mechanical Algebraic Variational Methods for Inelastic and Reactive Molecular Collisions," D. W. Schwenke, K. Haug, M. Zhao, D. G. Truhlar, Y. Sun, J. Z. H. Zhang, and D. J. Kouri, *Journal of Physical Chemistry* **92**, 3202-3216 (1988). (Proceedings of 1987 American Conference on Theoretical Chemistry)
- "Quantum Dynamics of Chemical Reactions by Converged Algebraic Variational Calculations," D. G. Truhlar, D. W. Schwenke, and D. J. Kouri, *Journal of Physical Chemistry* **94**, 7346-7352 (1990). (Invited Feature article)
- "From Force Fields to Dynamics: Classical and Quantal Paths," D. G. Truhlar and M. S. Gordon, *Science* **249**, 491-498 (1990). (invited article)
- "Control of Chemical Reactivity by Quantized Transition States," D. C. Chatfield, R. S. Friedman, D. W. Schwenke, and D. G. Truhlar, *Journal of Physical Chemistry* **96**, 2414-2421 (1992). (Invited Feature article)
- "Nonadiabatic Trajectories at an Exhibition," M. D. Hack and D. G. Truhlar, *Journal of Physical Chemistry A* **104**, 7917-7926 (2000). (Invited Feature article)

- "The Role of Collective Solvent Coordinates and Nonequilibrium Solvation in Charge Transfer Reactions," G. K. Schenter, B. C. Garrett, and D. G. Truhlar, *Journal of Physical Chemistry B* **105**, 9672-9685 (2001). (Invited Feature article)
- "The Incorporation of Quantum Effects in Enzyme Kinetics Modeling," D. G. Truhlar, J. Gao, C. Alhambra, M. Garcia-Viloca, J. Corchado, M. L. Sánchez, and J. Villà, *Accounts of Chemical Research* **35**, 341-349 (2002).
- "How Enzymes Work: Analysis by Modern Rate Theory and Computer Simulations," M. Garcia-Viloca, J. Gao, M. Karplus, and D. G. Truhlar, *Science* **303**, 186-195 (2004). (Review)
- "Introductory Lecture: Nonadiabatic Effects in Chemical Dynamics," A. W. Jasper, C. Zhu, S. Nangia, and D. G. Truhlar, *Faraday Discussions* **127**, 1-22 (2004). doi.org/[10.1039/B405601A](https://doi.org/10.1039/B405601A)
- "Non-Born-Oppenheimer Molecular Dynamics," A. W. Jasper, S. Nangia, C. Zhu, and D. G. Truhlar, *Accounts of Chemical Research* **39**, 99-106 (2006).
- "QM/MM: What Have We Learned, Where are We, and Where Do We Go from Here?" H. Lin and D. G. Truhlar, *Theoretical Chemistry Accounts* **117**, 185-199 (2007). (Feature article: Keynote paper in the Proceedings of the Tenth Electronic Computational Chemistry Conference) doi.org/10.1007/s00214-006-0143-z
- "Density Functionals with Broad Applicability in Chemistry," Y. Zhao and D. G. Truhlar, *Accounts of Chemical Research* **41**, 157-167 (2008).
- "A Universal Approach to Solvation Modeling," C. J. Cramer and D. G. Truhlar, *Accounts of Chemical Research* **41**, 760-768 (2008).
- "Applications and Validations of the Minnesota Density Functionals," Y. Zhao and D. G. Truhlar, *Chemical Physics Letters* **502**, 1-13 (2011). (invited Frontiers article)
- "The Quest for a Universal Density Functional: The Accuracy of Density Functionals Across a Broad Spectrum of Databases in Chemistry and Physics," R. Peverati and D. G. Truhlar, *Philosophical Transactions of the Royal Society A* **372**, 20120476/1-51 (2014). doi.org/10.1098/rsta.2012.0476 (part of a theme issue on "DFT for Physics, Chemistry and Biology").
- "Chemical Kinetics and Mechanisms of Complex Systems: A Perspective on Recent Theoretical Advances," S. J. Klippenstein, V. Pande, and D. G. Truhlar, *Journal of the American Chemical Society* **136**, 528-546 (2014). (invited Perspective Article) doi.org/10.1021/ja408723a
- "Quantum Mechanical Fragment Methods Based on Partitioning Atoms or Partitioning Coordinates," B. Wang, K. R. Yang, X. Xu, M. Isegawa, H. R. Leverentz, and D. G. Truhlar, *Accounts of Chemical Research* **47**, 2731-2738 (2014). (Special Issue: Beyond QM/MM: Fragment Quantum Mechanical Methods) dx.doi.org/10.1021/ar500068a
- "Explicit Polarization: A Quantum Mechanical Framework for Developing Next Generation Force Fields," J. Gao, D. G. Truhlar, Y. Wang, M. Mazack, P. Löffler, M. Provorse, and P. Rehak, *Accounts of Chemical Research* **47**, 2837-2845 (2014). dx.doi.org/10.1021/ar5002186 (Special Issue: Beyond QM/MM: Fragment Quantum Mechanical Methods)

- “The Importance of Ensemble Averaging in Enzyme Kinetics,” L. Masgrau and D. G. Truhlar, *Accounts of Chemical Research* **48**, 431-438 (2015).  
[dx.doi.org/10.1021/ar500319e](https://doi.org/10.1021/ar500319e) (invited contribution to special issue on Protein Motion in Catalysis)
- “Perspective: Kohn-Sham Density Functional Theory Descending a Staircase,” H. S. Yu, S. L. Li, and D. G. Truhlar, *Journal of Chemical Physics* **145**, 130901/1-23 (2016).  
[doi.org/10.1063/1.4963168](https://doi.org/10.1063/1.4963168) (invited perspective article)
- “Multiconfiguration Pair-Density Functional Theory: A New Way to Treat Strongly Correlated Systems,” L. Gagliardi, D. G. Truhlar, G. Li Manni, R. K. Carlson, C. E. Hoyer, and J. L. Bao, *Accounts of Chemical Research* **50**, 66-73 (2017). [doi.org/10.1021/acs.accounts.6b00471](https://doi.org/10.1021/acs.accounts.6b00471)
- “Variational Transition State Theory: Theoretical Framework and Recent Developments,” J. L. Bao and D. G. Truhlar, *Chemical Society Reviews* **46**, 7548-7596 (2017). (This article is part of the themed collection: Chemical Reaction Dynamics.)  
[doi.org/10.1039/C7CS00602K](https://doi.org/10.1039/C7CS00602K)
- “Computational Design of Functionalized Metal–Organic Framework Nodes for Catalysis,” V. Bernales, M. A. Ortuño, D. G. Truhlar, C. J. Cramer, and L. Gagliardi, *ACS Central Science* **4**, 5-19 (2018). (Outlook) [doi.org/10.1021/acscentsci.7b00500](https://doi.org/10.1021/acscentsci.7b00500)
- “Status and Challenges of Density Functional Theory,” P. Verma and D. G. Truhlar, *Trends in Chemistry* **2**, 302-318 (2020). (Feature Review –First Anniversary Issue: Laying the Groundwork for the Future) [doi.org/10.1016/j.trechm.2020.02.005](https://doi.org/10.1016/j.trechm.2020.02.005)
- “Diabatic States of Molecules,” Y. Shu, Z. Varga, S. Kanchanakungwankul, L. Zhang, and D. G. Truhlar, *Journal of Physical Chemistry A* **126**, 992-1018 (2022). (Invited Feature Article) [doi.org/10.1021/acs.jpca.1c10583](https://doi.org/10.1021/acs.jpca.1c10583)
- “Electronic Structure of Strongly Correlated Systems: Recent Developments in Multiconfiguration Pair-Density Functional Theory and Multiconfiguration Nonclassical-Energy Functional Theory,” C. Zhou, M. R. Hermes, D. Wu, J. J. Bao, R. Pandharkar, D. S. King, D. Zhang, T. R. Scott, A. O. Lykhin, L. Gagliardi, and D. G. Truhlar, *Chemical Science* **13**, 7685-7706 (2022) (invited Perspective article) [doi.org/10.1039/D2SC01022D](https://doi.org/10.1039/D2SC01022D)

## TRAINING AND RESEARCH ADVISING

### Postdoctoral research scholars and research associates sponsored and supervised:

- |                                |                                 |
|--------------------------------|---------------------------------|
| 1. Richard Smith, 1971-72      | 10. Jack Lauderdale, 1984-85    |
| 2. Bruce Garrett, 1977-80      | 11. David Schwenke, 1985-87     |
| 3. Kunizo Onda, 1978-80        | 12. Carmay Lim, 1986            |
| 4. Alan Isaacson, 1980-81      | 13. Thomas Georgian, 1986-87    |
| 5. Steven Valone, 1980-82      | 14. Gene Hancock, 1986-87       |
| 6. Najib Abusalbi, 1981-82     | 15. Tomi Joseph, 1986-88        |
| 7. Sachchida Rai, 1982-83      | 16. Mirjana Mladenovic, 1987-88 |
| 8. Grazyna Staszewska, 1982-83 | 17. Philippe Halvick, 1988-89   |
| 9. Franklin Brown, 1983-85     | 18. Da-hong Lu, 1989-91         |

19. Angels Gonzalez-Lafont, 1989-91 (Fulbright Scholarship)
20. Ronald S. Friedman, 1989-91
21. Thanh Truong, 1990
22. Gregory Tawa, 1990-93
23. Robert Topper, 1990-92
24. Qi Zhang, 1991-92
25. Melissa Reeves, 1991-93
26. Kathleen Kuhler, 1993-94
27. Ivan Rossi, 1993-95
28. Candee Chambers, 1994-96
29. Kiet Nguyen, 1994-96
30. Xavier Assfeld, 1994-96
31. Elena Laura Coitiño, 1995–97
32. Maria Topaler, 1996-98
33. Jose Corchado, 1996-98 (Fulbright Scholar)
34. Orlando Robert-Neto, 1996-97
35. Jordi Villà, 1998
36. Maria Sanchez, 1998-99
37. Yongho Kim, 1999-2000
38. Hisao Nakamura, 2000-2002
39. Liqiang Wei, 2000-2001
40. Titus Albu, 2000-2002
41. Przemek Staszewski, 2002-2003, 2004
42. Chaoyuan Zhu, 2002-2005
43. Hai Lin, 2003-2005
44. Ahren Jasper, 2003-2005
45. Joanna Kryven (formerly Osanna Tishchenko), 2005-2017
46. Rosendo Valero, 2005-2009
47. Zhenhua Li, 2005-2007
48. Mark Iron, 2005-2007
49. Yan Zhao, 2005-2008
50. Yuan Zhang, 2005-2006
51. Divesh Bhatt, 2005-2006
52. Andreas Heyden, 2006-2007
53. Jingjing Zheng, 2006-2015
54. Anastassia Sorkin, 2006-2007
55. David Bonhommeau, 2006-2008
56. Masahiro Higashi, 2007-2009
57. Meiyu Zhao, 2007-2008
58. Steven Mielke, 2008-2017
59. Manjeera Mantina, 2008-2009
60. Boris Averkiev, 2009-2012
61. Ruifang Li, 2009-10
62. John Alecu, 2009-2012
63. Miho Isegawa, 2009-2013 (joint with J. Gao for 2009-2011)
64. Anant Kulkarni, 2010-2012
65. Roberto Peverati, 2010–2012
66. Xuefei Xu, 2010–2015
67. Prasenjit Seal, 2011–2015
68. Yuliya Paukku, 2011–2018
69. Rubén Meana-Pañeda, 2011-2016
70. Gbenga Oyedepo, 2011-13
71. Zoltan Varga, 2012-2015, 2016-present
72. Bo Wang, 2013-2015
73. Laura Fernandez, 2013-2016
74. Max Makeev, 2014-2015
75. Wei Lin, 2014-2015
76. Shuping Huang, 2014-2016
77. Wei-Guang Liu, 2014-2017
78. Guoliang Song, 2015-2016
79. Yinan Shu, 2016-present
80. Xin-Ping Wu, 2016-2019 (joint with L. Gagliardi in 2016-2018)
81. Sijia Dong, 2017-2019 (joint with L. Gagliardi, 2018-2019)
82. Pragya Verma, 2017-2018
83. Indrani Chaudhuri, 2018-2020
84. Chen Zhou, 2018-2021
85. Dihua Wu, 2019-present
86. Jie Bao, 2021-present
87. Farideh Badichi, 2021- present
88. Maryam Mansori, 2022- present

joint supervision with Christopher J. Cramer:

89. Joey W. Storer, 1993-94
90. Tianhai (Tony) Zhu, 1996-98
91. Jiabo Li, 1997-99
92. Kevin Silverstein, 1998
93. James Xidos, 1999-2001
94. Benjamin Lynch, 2003-2005
95. Pablo Jaque, 2005-2006
96. Alek Marenich, 2006-2016
97. Ryan Olson, 2006-2007
98. Jingyun Ye, 2016-2020 (joint with L. Gagliardi, 2016-2018)

joint supervision with Jiali Gao:



99. Tina Poulsen, 2001-2002  
100. Jingzhi Pu, 2004-2005

101. S'moorthi Nachimuthu, 2010–  
2011

joint supervision with J. Ilja Siepmann:

102. Hannah Leverentz, 2012-2013

joint supervision with Laura Gagliardi:

103. Andrew Sand, 2015-2018  
104. Kamal Sharkas, 2015-2018  
105. Bo Yang, 2016-2019

**Graduate thesis supervision:**

Chemistry, Ph.D.

- 1 Robert W. Numrich, 1974
- 2 James W. Duff, 1975
- 3 Nancy Mullaney Harvey, 1979
- 4 Devarajan Thirumalai, 1981
- 5 Todd Cameron Thompson, 1984
- 6 David Winston Schwenke, 1985
- 7 Rozeanne Steckler, 1986
- 8 Joni C. Gray, 1989
- 9 Susan C. Tucker, 1989
- 10 Thanh N. Truong, 1989
- 11 Paul N. Day, 1991
- 12 David C. Chatfield, 1991
- 13 Yi-Ping Liu, 1993
- 14 Michael Unekis, 1993
- 15 Vasilios Melissas, 1993
- 16 Gillian Lynch, 1993
- 17 Wei-Ping Hu, 1995
- 18 William Necochea, 1995
- 19 Steven Wonchoba, 1997
- 20 Thomas Allison, 1997
- 21 Eric Schwegler, 1998
- 22 Gregory Hawkins, 1998
- 23 Sutjano Jusuf, 1999
- 24 Patton Fast, 2000
- 25 Michael Hack, 2000
- 26 Benjamin Lynch, 2003
- 27 Ahren Jasper, 2003
- 28 Jingzhi Pu, 2004
- 29 Jason Thompson, 2004 (joint adviser with C. J. Cramer)
- 30 Vanessa Audette Lynch, 2005
- 31 Yan Zhao, 2005
- 32 Arindam Chakraborty, 2005
- 33 Shikha Nangia, 2006
- 34 Nathan Schultz, 2006
- 35 Casey Kelly, 2007 (joint adviser with C. J. Cramer)
- 36 Ben Ellingson, 2007
- 37 Erin Dahlke, 2007
- 38 Adam Chamberlin, 2008 (joint adviser with C. J. Cramer)
- 39 Wangshen Xie, 2008 (joint adviser with J. Gao)
- 40 Ewa Papajak, 2012
- 41 Tao Yu, 2012
- 42 Bo Wang, 2013
- 43 Haoyu Yu, 2016
- 44 Kaining Duanmu, 2016
- 45 Shaohong Li, 2017
- 46 Pragya Verma, 2017
47. Chad Hoyer, 2017 (joint adviser with L. Gagliardi)
48. Junwei Lucas Bao, 2018

49. Kelsey Parker, 2020
50. Jie Bao, 2021

Chemistry, M. S.

- 1 Joseph Abdallah, Jr., 1974
- 2 Maynard A. Brandt, 1975
- 3 David Cochrane, 1990
- 4 Daniel Theis, 2006
- 5 Hadi Dinpajoo, 2010 (joint adviser with J. I. Siepmann)
- 6 Run Li, 2011
- 7 Bo Wang, 2009
- 8 Luke Fiedler, 2009
- 9 Raphael Ribeiro, 2012 (joint adviser with C. J. Cramer)
- 10 Kaining Duanmu, 2013
- 11 Haoyu Yu, 2013
- 12 Pragma Verma, 2013
- 13 Shaohong Li, 2013
- 14 Chad Hoyer, 2014 (joint adviser with L. Gagliardi)
- 15 Junwei (Lucas) Bao, 2014
16. Kelsey Parker, 2015
- 17 Jie Bao, 2017
- 18 Siriluk Kanchanakungwankul, 2018
- 19 Jiaxin Ning, 2019
- 20 Dayou Zhang, 2019
- 21 Suman Bhaumik, 2021

Chemical Physics, Ph. D.

- 1 Rex T. Skodje, 1983
- 2 Carmay Siow Chiow Lim, 1984
- 3 Kenneth Haug, 1987
- 4 Meishan Zhao, 1989
- 5 Xin Gui Zhao, 1990
- 6 Steven Mielke, 1995
- 7 Yao-Yuan (John) Chuang, 1999
- 8 Jay Srinivasan, 1999
- 9 Yuri Volobuev, 2000
- 10 Tiqing Liu, 2000
- 11 Hannah Leverentz, 2012
- 12 Sijie (Andy) Luo, 2014
- 13 Ke R. Yang, 2014

Chemical Physics, M. S.

- 1 Haozhe Dong, 1990
- 2 Jianhua Xing, 1998
- 3 Hannah Leverentz, 2009
- 4 Ke Yang, 2010
- 5 Sijie (Andy) Luo, 2011
- 6 Mayank Dodia, 2017

Medicinal Chemistry, Ph. D.

- 1 Brian White, 2009 (co-advised with C. R. Wagner)

## Current Ph.D. students

- 1 Luke Fiedler, Chemistry (part-time))
- 2 Siriluk Kanchanakungwankul, Chemistry, entered 2017
- 3 Jiaxin Ning, Chemistry, entered 2018
- 4 Dayou Zhang, Chemistry, entered 2018
- 5 Suman Bhaumik, entered 2019
6. Aiswarya M. Parameswaran, entered 2021

**Undergraduate research students:**

1. James Sorenson, 1971
2. Jean Merrick, 1974–75
3. Radley Olson, 1974
4. Richard Partridge, 1975
5. Ruth Poling, 1975
6. William Tarara, 1975
7. Laura Clemens, 1976
8. Charles Horowitz, 1977
9. Dale Zurawski, 1977
10. Gerald Fraser, 1978
11. Nancy Kilpatrick, 1978
12. Rex Skodje, 1978
13. Eve Zoebisch, 1979
14. Roger Grev, 1979–80
15. Alan Magnuson, 1979
16. Dmitry Altshuller, 1980
17. Brian Reid, 1980
18. Tonny Nam, 1981
19. Keith Runge, 1982
20. Susan Tucker, 1983–84
21. Kenneth Dykema, 1984
22. Paul Rejto, 1985
23. Beth Sponholtz, 1988
24. David Maurice, 1989
25. Gregory Taylor, 1990
26. Jason Goepfing, 1991
27. Dean Briesemeister, 1992–93
28. Martine Kalke, 1993
29. Michael Zhen Gu, 1994–96
30. Michael Hack, 1994
31. Yuri Volobuev, 1994
32. Andrew Welch, 1994
33. Zoran Svetlicic, 1995
34. Steven Clayton, 1996
35. Molli Noland, 1996
36. Jason Lang, 1997-98
37. Joe Danzer, 1997
38. Darrell Hurt, 1997
39. Derek Dolney, 1997-98
40. Brent Fischer, 1998
41. Mala Radhakrishnan, 1998
42. Jocelyn Rodgers, 1998-99
43. Maegan Harris, 1999
44. Thomas F. Miller III, 1999
45. Christine Tratz (now Aikens), 1999
46. Nathan Schultz, 2000
47. Timothy Sonbuchner, 2000
48. Amanda Wensman, 2000
49. Sam Stechman, 2001
50. Amber Nolan, 2001-2002
51. Amos Anderson, 2001-2003
52. Brian Schmitz, 2002
53. Jill Leas, 2003
54. Kara Johnson, 2005
55. Ian Haken, 2005
56. Thomas J. Preston, 2005
57. Natalie Elmasry, 2005-07, joint with C. Cramer
58. Carly Sodahl, 2005-06
59. Michael W. Collins, 2006
60. Michelle Orthmeyer, 2006
61. Jacob Sirek, 2006, joint w/ C. Cramer)
62. Hannah Leverentz, 2006-07
63. Jonathan Young, 2007
64. Alex Kozin, 2007
65. Robert Berscheid Jr. 2008-09
66. Di Wu, 2008-2009
67. Raphael Ribiero 2009-10, joint with C. Cramer
68. Antonio Oliviero Filho, 2009
69. Sarah Kragt, 2009-10
70. Steve Jerome, 2009
71. Wendu Ding, 2009, joint w/ C. Cramer

- |                                                  |                                                   |
|--------------------------------------------------|---------------------------------------------------|
| 72. Michelle Lenz, 2010                          | 81. Kelsey Parker, 2014, joint with L. Gagliardi  |
| 73. Duy P. Hua 2010                              | 82. Siriluk Kanchanakungwankul, 2016-2017         |
| 74. Gillian Shaw, 2011                           | 83. Hirbod Heidari, 2017                          |
| 75. Jeremy Tempkin, 2011                         | 84. Hung Vuong, 2018                              |
| 76. Abir Majundar, 2012-13, joint with C. Cramer | 85. Kevin Huang, 2018-19                          |
| 77. Helena Qi, 2012                              | 86. Erica Mitchell, 2019, joint with L. Gagliardi |
| 78. Tiago Dominguez, 2012-13                     | 87. Lyuben Borislavov, 2019                       |
| 79. Chad Hoyer, 2012, joint with L. Gagliardi    | 88. Darya Snitvets, 2021                          |
| 80. He Ma, 2014                                  | 89. Bhavnesh Jangid, 2022                         |

I have 67 publications with undergraduate coauthors (47 different undergraduates).

**Outside examiner, Ph.D. Theses:** John Scott Carley, University of Waterloo (Canada), 1978; Margot Mandy, University of Toronto (Canada), 1991

Outside reader, Ph.D. Thesis:

Stephen Malcolm McPhail, University of Sydney (Australia), 1980;  
 Christofer Tautermann, University of Innsbruck (Austria), 2002;  
 Balkrishna P. Shah, The Maharaja Sayajirao University of Baroda (Vadodara, India), 2003;  
 Pradeep Kumar, Indian Institute of Technology, Kanpur, 2012

Visiting collaborators and students with extended stays:

Prof. Mark S. Gordon, 1985-86 (sabbatical)  
 John Zhang, 1986  
 Prof. Grazyna Staszewska, 1986, 1990, 2002-2003 (sabbatical), 2004, 2005  
 Yaakov Shima, 1986  
 Yici Zhang, 1987  
 Yan Sun, 1987  
 Prof. Antonio J. C., 1987 (sabbatical), 2011, 2012  
 Omar Sharafeddin, 1987  
 Prof. Don Kouri, 1987-88  
 Rex Skodje, 1988  
 Kim Baldrige, 1988  
 Csilla Duneczky, 1988  
 Prof. Jan Linderberg, 1988  
 Rozeanne Steckler, 1988  
 Bruce C. Garrett, 1988, 1992, 1994  
 Chin-hui Yu, 1989  
 Prof. Brian Sutcliffe, 1990  
 David Schwenke, 1990, 1991, 1993-94  
 Christopher Cramer, 1990-91 (postdoctoral)  
 Prof. Ahmed S. Shalabi, 1991  
 Prof. Charles Jackels, 1993-94 (sabbatical)  
 Jose Corchado, 1994  
 Jordi Villa, 1995, 1996-1997  
 Prof. Steven Bachrach, 1997 (sabbatical)

Prof. Brian Williams, 1997 (sabbatical)  
Prof. Joaquin Espinosa-Garcia, 1997  
Laura Masgrau, 1999  
Prof. Antonio Fernandez-Ramos, 2000, 2003, 2004, 2005, 2017, 2018  
Prof. Piotr Paneth, 2000-2001 (sabbatical)  
Prof. Przemek Staszewski, 2002-2003, 2004, 2005  
Prof. Joseph Brom, 2002-2003 (sabbatical)  
John Keith, 2002  
Agnieszka Dybala-Defratyka, 2002  
Iva Tatic, 2002  
Prof. Larry Pratt, 2003, 2004  
Prof. Keith Kuwata, 2003-2004 (sabbatical)  
Luis Campos, 2003  
Prof. Clayton Spencer, 2004-2005  
Nuria Gonzalez, 2004, 2005  
Javier Ruiz Pernia, 2004, 2005  
Jaiyun Pang, 2004-2005  
Prof. Masato Nakamura, 2005  
Shivangi Nangia, 2005  
Prof. Sonia Ilieva, 2005-2006 (Fulbright Fellow)  
Michal Rostkowski, 2005  
Prof. Jonathan Smith, 2006-07 (sabbatical)  
Neil Young, 2006  
Yousung Jung, 2007  
Peifung Su, 2007  
Rubén Meana-Pañeda, 2008  
Prof. Yongho Kim, 2008-09 (sabbatical)  
Hai Lin, 2009 (joint with IMA)  
Bastiaan Braams, 2009  
Orlando Roberto-Neto, 2009-2010  
Varinia Bernales, 2011-12  
Amrit Jalan, 2012  
Wenjing Zheng, 2012-2014  
Pattrawan Sripa, 2014  
Prof. Xiao He, 2014, 2015  
Xiaoyu Li, 2015-2016  
Prof. Xin Zhang, 2015-2016  
Prof. Bo Long, 2015-2016  
Andrey Pershin, 2016  
Prof. Xuefei Xu, 2017  
Lili Xing, 2016-2017  
Wanqiao Zhang, 2016-2017  
Linyao Zhang, 2017-2019  
Prof. Yan Zhao, 2018  
Lu G. Gao, 2018-2019  
Junjun Wu, 2019  
Shuhang Li, 2019  
Xu Cai, 2019-2020  
Xiaozhe Fan, 2019-2020  
Rui Ming Zhang, 2019-2020  
Yao-Yuan (John) Chuang, 2022

---

**Commercialized Technology Transfer**

Licensed Software, *MNSOL Database*, University of Minnesota Office for Technology Commercialization 2008

Licensed Software, *AMSOL*, University of Minnesota Office for Technology Commercialization 2005

**Symposia organized at American Chemical Society meetings:**

1. Potential Energy Surfaces and Dynamics Calculations, Symposium at National Meeting of the American Chemical Society, Las Vegas, 1980, organizer
2. Resonances in Electron-Molecule Scattering, van der Waals Molecules, and Reactive Chemical Dynamics, Symposium at National Meeting of American Chemical Society, St. Louis, 1984, organizer
3. ACS Division of Industrial and Engineering Chemistry Symposium on Supercomputer Research in Chemistry and Chemical Engineering, Minneapolis, 1987, co-organizer
4. Classical and Quantal Simulations for Reactive and Solvation Dynamics and their Critical Experimental Tests, Symposium at National Meeting of the American Chemical Society, Boston, 1990, co-organizer
5. Structure and Reactivity in Aqueous Solution, Symposium at National Meeting of American Chemical Society, San Diego, California, 1994, co-organizer
6. Symposium on The Role of Electrostatics in Chemistry, National Meeting of the American Chemical Society, 31 papers, co-organizer (supported in part by the ACS Petroleum Research Fund), Sept. 13-17, 1997, Las Vegas, co-organizer
7. Symposium on Transition State Modeling for Catalysis, American Chemical Society, Division of Computers in Chemistry, National Meeting of the American Chemical Society, 40 lecturers from 13 countries, March 29-April 2, 1998, Dallas, co-organizer
8. Symposium on Electronically Nonadiabatic Processes in Gaseous, Cluster, and Condensed Media, National Meeting of the American Chemical Society, New Orleans, Louisiana, August 23-26, 1999, co-organizer
9. Computational Chemistry at the Interface Symposium, Great Lakes Regional Meeting, June 2-4, 2002, Minneapolis, 18 speakers from 11 states and 2 countries; co-organizer and chair
10. Computational Electrochemistry, Boston National ACS Meeting, August 2007, 25 speakers from six countries, co-organizer with Michel Dupuis.
11. Symposium on Computational Chemistry for Geochemistry, sponsored by Geochemistry Division of the ACS, National Meeting of the American Chemical Society, San Diego, California, 2012, co-organizer, speakers from 11 states and four countries
12. Combustion Chemistry Symposium, New Orleans National ACS Meeting, April 7-8, 2013, co-organizer 16 invited speakers and 8 contributed papers. Also at same meeting: Kinetics of Combustion Symposium, April 10, 2013, 17 contributed papers

**Symposium organized at American Physical Society meeting:**

1. Recent Advances in Density Functional Theory and Applications in Chemical Physics, Symposium at March National Meeting of the American Physical Society, Baltimore, March 14-18, 2016, lead organizer

**Other national and international conferences and workshops organized and co-organized:**

1. Symposium on Vibrational Spectroscopy and Chemical Structures, in Honor of Bryce Crawford, Minneapolis, 1983, co-organizer
2. Institute for Mathematics and Its Applications Workshop on Atomic and Molecular Structure and Dynamics, University of Minnesota, 1987, organizer

3. NATO Advanced Research Workshop on Supercomputer Algorithms for Reactivity, Dynamics, and Kinetics of Small Molecules, Colembella di Perugia, Italy, 1988, organizing committee
4. Minnesota Supercomputer Institute Workshop on Practical Iterative Methods for Large-Scale Computations, Minneapolis, 1988, cochairman
5. Minnesota Supercomputer Institute Symposium on Supercomputer Protein Chemistry, 1989, organizer
6. Minnesota Supercomputer Institute Workshop on Domain-Based Parallelism and Problem Solving Decomposition Methods in Computational Science and Engineering, sponsored by Minnesota Supercomputer Institute in conjunction with the Supercomputer Activity Group of the Society for Industrial and Applied Mathematics, 18 lectures, 74 registrants from 18 states and 7 countries, April 25–26, 1994, Minneapolis, co-organizer
7. International Symposium on Computational Molecular Dynamics, cosponsored by University of Minnesota Supercomputer Institute, Computers in Chemistry Division of American Chemical Society, Division of Computational Physics of the American Physical Society, and Physical Chemistry Division of the American Chemical Society, 25 speakers, 105 posters, 185 registrants from 27 states and 13 countries, October 24–26, 1994, Minneapolis, organizer
8. Workshop on Multiparticle Quantum Scattering with Applications to Nuclear, Atomic, and Molecular Physics, Institute for Mathematics and its Applications, University of Minnesota, 20 lectures, 36 registrants from 11 countries, June 7–16, 1995, Minneapolis, co-organizer
9. Minnesota Supercomputer Institute/IBM International Conference on Parallel Computing, 1996, organizing committee chair
10. Institute for Mathematics and its Applications/Minnesota Supercomputer Institute, Workshop on Rational Drug Design, co-organizer (with W. Jeffrey Howe, Jeffrey M. Blaney, Richard Dammkoehler, and Anton J. Hopfinger), April 7-11, 1997.
11. First Annual University of Minnesota Computational Neuroscience Symposium, sponsored by Computational Neuroscience Program of the University of Minnesota, co-organizer, Oct. 7-8, 1999
12. 2001 Pasadena Workshop on Quantum Reaction Dynamics in honor of Aron Kuppermann's 75<sup>th</sup> Birthday, Jan. 10-13, 2001, Pasadena, CA, co-organizer.
13. CNER-MSI Nanosimulation Workshop Center for NanoEnergetics Research - Minnesota Supercomputing Institute, August 26, 2002; 9 speakers from six states and two countries; organizer and chair
14. Advances in Quantum Chemistry: Interfacing Electronic Structure with Dynamics (Satellite Symposium of the International Congress of Quantum Chemistry), June 20-22, 2012, Minneapolis, co-organizer, 30 speakers from 12 states and six countries, 46 posters, 99 registered attendees

**Regional conferences co-organized:**

1. Thirteenth Annual Midwest Theoretical Chemistry Conference, Minneapolis, 1980, co-chaired
2. Midwest Theoretical Chemistry Conference, sponsored by University of Minnesota Supercomputer Institute, Army High Performance computing research Center, Cray, Inc., Compaq, IBM, and SGI, 144 attendees from fifteen states, Canada and Australia, Oct. 5-6, 2001, Minneapolis, co-chair

**Other national and international conferences and workshops conference service:**

1. Conference on the Dynamics of Molecular Collisions, Treasurer, 1989-2011
2. Supercomputing Conference 2000 (sponsored by Association for Computing Machinery and IEEE Computer Society), Dallas, Texas, Nov. 4-10, 2000, Technical Papers Committee



3. XIIth International Workshop on Quantum Atomic and Molecular Tunneling in Solids (QAMTS 2003), University of Florida, Gainesville June 22 - 25, 2003, advisory planning committee
4. Congress of the International Society for Theoretical Chemical Physics, Vancouver CANADA, July 19-24th 2008, Scientific Committee
5. 10th Congress of the World Association of Theoretical and Computational Chemists (WATOC 2014), Santiago, Chile, October 5-10, 2014, International Scientific Committee