

May 26, 2025

## DONALD G. TRUHLAR

### Personal and contact information

Birth: Feb. 27, 1944, Chicago, IL

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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)

John Stauffer Fellow, National Defense Graduate Fellow, Woodrow Wilson Foundation Fellow

### Appointments

University of Minnesota:

Department of Chemistry

Member of Graduate Faculty, 1969-present

Assistant Professor, 1969-72

Associate Professor, 1972-76

Professor, 1976-2006

George Taylor Institute of Technology Professor, 1993-1998

Institute of Technology/CSE Distinguished Professor, 1998-present

Lloyd H. Reyerson Professor, 2002-2006

Regents Professor, 2006-

Director of Graduate Studies, 1986-88

Chemical Physics Program

Member of Graduate Faculty, 1969-present

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

Minnesota Supercomputing Institute

Fellow, 1985-

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

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

### **Direction of nationally funded multi-university centers**

Computational Neuroscience Program (National Institutes of Health)  
Co-Director, 1998-2009  
Center for the Processing and Behavior of Nanoenergetic Materials (U. S. Army)  
Director, 2004-2007  
Research Tools Design Consortium for Computation Chemistry (U. S. Navy)  
Director, 2005-2009  
Nanoporous Materials Genome Center (U. S. Department of Energy)  
Deputy Director, 2018-2022

### **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.

[pubs.acs.org/page/jctcce/vi/truhlar.html](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.

Commemorative Special Issue of *Molecules* Honoring Professor Donald Truhlar, 2022

[www.mdpi.com/journal/molecules/special\\_issues/Donald\\_Truhlar](http://www.mdpi.com/journal/molecules/special_issues/Donald_Truhlar)

Joseph O. Hirschfelder Prize in Theoretical Chemistry for 2023

“many important and broad contributions to theoretical chemistry in electronic structure calculations, variational transition state theory, solvation models, and quantum mechanical scattering theory. His work has significantly advanced our understanding of chemical dynamics and spectroscopy.”

ACS Computers in Chemistry Division Symposium in Honor of Donald G. Truhlar’s 80th Birthday, 2024

“Prof. Don Truhlar has made extensive seminal contributions in theoretical/computational chemistry and chemical physics. His works have influenced various fields from reaction dynamics to density functional theory, from multiscale modeling to solvation, from catalysis to combustion, from atmospheric chemistry to environmental issues, from nanoparticles to photochemistry, from enzymes to solid-state materials, and many more. Such broad impacts by one individual theoretical chemist on so many frontiers in chemistry, physics, and biology, are rare, if not unique. This symposium will celebrate Don’s remarkable and continuing career in science on his 80th birthday and will feature groundbreaking computational chemistry research from Don and his colleagues throughout academia and industry across the world.” ACS National Meeting, August 18-19, 2024, Denver. The symposium featured 21 talks by collaborators and former students and postdocs: Yihan Shao, Rubén Meana-Pañeda, Jiali Gao, Hai Lin, Shikha Nangia, Laura Gagliardi, Jingjing Zheng, Arindam Chakraborty, Andreas Heyden, David Schwenke, Hua Guo, Sijia Dong, Roland Lindh, Yan Zhao, Xiaosong Li, Jingzhi Pu, Ahren Jasper, Lucas Bao, Jingyun Ye, Ilja Siepmann, and Ben Janesko.

Caltech’s Distinguished Alumni Award, 2025

“in recognition of your advances in theoretical and computational chemistry”. The Distinguished Alumni Award is the highest honor presented by Caltech to its graduates.

**“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”

60th Birthday Symposium, University of Minnesota, 2004

international symposium organized by Chris Cramer, Bruce Garrett, Dave Thirumalai, and Thanh Truong

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 multidimensional tunneling methods  
 Converged quantum dynamics for chemical kinetics, scattering, and resonances  
 Quantum mechanical and semiclassical methods for photochemical dynamics  
 Universal solvation models, including SMD and SM12  
 Vibrational anharmonicity  
 Minnesota functionals for Kohn-Sham density functional theory  
 Multi-configuration nonclassical-energy 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 include:

- 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
- the study of photoactivated processes, including excitation energies, coupled potential energy surfaces and their couplings, and multi-state dynamics
- 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
- quantum mechanical treatment of vibrations, including vibrational configuration interaction, multistructural effects, and torsions
- transition metal chemistry for catalysis and magnetic properties
- metal–organic frameworks for catalysis
- new methods for path integral calculations in quantum mechanical statistical mechanics and applications to vibrational-rotational free energies
- battery development: structure, electromotive force, capacity, and transport

**Bibliography**

1392 journal articles, 89 book chapters, 14 books edited.

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

**Citation Statistics**

Statistics from Google Scholar, May 26, 2025:

Number of citations: 251,997. h-index: 202. i10 index: 1426.

Citations since 2020: 83,862.

articles with 1000 or more citations. 32

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

Statistics from Clarivate Web of Science, May 26, 2025:

Number of citations: 200,761 in 101,731 articles. h-index: 178.

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

Listed by Clarivate as *Highly Cited Researcher*

Based on statistics collected on 11/21/2023 for the 2023 Edition of the

Research.com Ranking of Top Scientists in the field of Chemistry:

<https://research.com/scientists-rankings/chemistry>, Professor Truhlar ranked 6th in the world and 3rd in United States. The only theorist in the world ranked higher was J. Nørskov of Denmark.

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

Dec. 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 supervision**

Number of research students:

Undergraduate: 91 (68 publications with 48 different undergraduate coauthors)

Graduate: 70 completed Ph.D. or both Ph. D. and M. S., 12 completed with M. S., 1 currently working toward Ph. D.

Postdoctoral: 107

**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:***

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

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;

National meeting 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 Editor, 2012-present.

Associate Editor:

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

Editorial Boards and Advisory Editorships:

*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, 1993-2018

*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, 2003-2023 (was called *Central European Journal of Chemistry* from 2003 to 2014)  
*Journal of Chemical Theory and Computation* (published by ACS), Advisory Board, 2004-2022  
*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: 92 (72 publications with 52 different undergraduate coauthors)
- Graduate: 67 completed Ph.D. or both Ph. D. and M. S., 12 completed with M. S., 3 currently working toward Ph. D.
- Postdoctoral: 107

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

Fellowships (since 2011) awarded to graduate 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

"History of H<sub>3</sub> Kinetics," D. G. Truhlar and R. E. Wyatt, in *Annual Review of Physical Chemistry*, Vol. 27, edited by B. S. Rabinovitch (Annual Reviews, Inc., Palo Alto, California, 1976), pp. 1-43. (invited front piece)

"Variational Transition-State Theory," D. G. Truhlar and B. C. Garrett, *Accounts of Chemical Research* **13**, 440-448 (1980). doi.org/10.1146/annurev.pc.35.100184.001111

"The Current Status of Transition State Theory," D. G. Truhlar, W. L. Hase, and J. T. Hynes, *Journal of Physical Chemistry* **87**, 2664-2682 (1983). doi.org/10.1021/j100238a003 (invited front piece for Henry Eyring Dedicatory Issue)

"Variational Transition State Theory," D. G. Truhlar and B. C. Garrett, in *Annual Review of Physical Chemistry*, Vol. 35, edited by B. S. Rabinovitch, J. M. Schurr, and H. L. Strauss (Annual Reviews, Inc., Palo Alto, California, 1984), pp. 159-189.  
doi.org/10.1146/annurev.pc.35.100184.001111

- “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)
- “Current Status of Transition State Theory,” D. G. Truhlar, B. C. Garrett, and S. J. Klippenstein, *Journal of Physical Chemistry* **100**, 12771-12800 (1996). doi.org/10.1021/jp953748q (invited article for Centennial Issue of journal)
- "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).
- "Quantum Mechanical Methods for Enzyme Kinetics," J. Gao and D. G. Truhlar, in *Annual Review of Physical Chemistry*, Vol. 53, edited by S. R. Leone, P. Alivasatos, and A. E. McDermott (Annual Reviews, Inc., Palo Alto, CA, 2002), pp. 467-505.
- “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 (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 (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

“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

“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

“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

“Multiconfiguration Pair-Density Functional Theory,” P. Sharma, J. J. Bao, D. G. Truhlar, and L. Gagliardi, in *Annual Review of Physical Chemistry*, Vol. 72, pages 541-564 (2021). https://doi.org/10.1146/annurev-physchem-090419-043839

“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

“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/1039/D2SC01022D

“Decoherence and its Role in Electronically Nonadiabatic Dynamics,” Y. Shu and D. G. Truhlar, *Journal of Chemical Theory and Computation* **19**, 380-395 (2022). (invited Perspective article) doi.org/10.1021/acs.jctc.2c00988

## TRAINING AND RESEARCH ADVISING

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

- |   |   |
|---|---|
| 1. Richard Smith, 1971-72                                   | 33. Jose Corchado, 1996-98 (Fulbright Scholar)          |
| 2. Bruce Garrett, 1977-80                                   | 34. Orlando Robert-Neto, 1996-97                        |
| 3. Kunizo Onda, 1978-80                                     | 35. Jordi Villà, 1998                                   |
| 4. Alan Isaacson, 1980-81                                   | 36. Maria Sanchez, 1998-99                              |
| 5. Steven Valone, 1980-82                                   | 37. Yongho Kim, 1999-2000                               |
| 6. Najib Abusalbi, 1981-82                                  | 38. Hisao Nakamura, 2000-02                             |
| 7. Sachchida Rai, 1982-83                                   | 39. Liqiang Wei, 2000-01                                |
| 8. Grazyna Staszewska, 1982-83                              | 40. Titus Albu, 2000-02                                 |
| 9. Franklin Brown, 1983-85                                  | 41. Przemek Staszewski, 2002-03, 2004                   |
| 10. Jack Lauderdale, 1984-85                                | 42. Chaoyuan Zhu, 2002-05                               |
| 11. David Schwenke, 1985-87                                 | 43. Hai Lin, 2003-05                                    |
| 12. Carmay Lim, 1986  | 44. Ahren Jasper, 2003-05                               |
| 13. Thomas Georgian, 1986-87                                | 45. Joanna Kryven (formerly Osanna Tishchenko), 2005-17 |
| 14. Gene Hancock, 1986-87                                   | 46. Rosendo Valero, 2005-09                             |
| 15. Tomi Joseph, 1986-88                                    | 47. Zhenhua Li, 2005-07                                 |
| 16. Mirjana Mladenovic, 1987-88                             | 48. Mark Iron, 2005-07                                  |
| 17. Philippe Halvick, 1988-89                               | 49. Yan Zhao, 2005-08                                   |
| 18. Da-hong Lu, 1989-91                                     | 50. Yuan Zhang, 2005-06                                 |
| 19. Angels Gonzalez-Lafont, 1989-91 (Fulbright Scholarship) | 51. Divesh Bhatt, 2005-06                               |
| 20. Ronald S. Friedman, 1989-91                             | 52. Andreas Heyden, 2006-07                             |
| 21. Thanh Truong, 1990                                      | 53. Jingjing Zheng, 2006-15                             |
| 22. Gregory Tawa, 1990-93                                   | 54. Anastassia Sorkin, 2006-07                          |
| 23. Robert Topper, 1990-92                                  | 55. David Bonhommeau, 2006-08                           |
| 24. Qi Zhang, 1991-92                                       | 56. Masahiro Higashi, 2007-09                           |
| 25. Melissa Reeves, 1991-93                                 | 57. Meiyu Zhao, 2007-08                                 |
| 26. Kathleen Kuhler, 1993-94                                | 58. Steven Mielke, 2008-17                              |
| 27. Ivan Rossi, 1993-95                                     | 59. Manjeera Mantina, 2008-09                           |
| 28. Candee Chambers, 1994-96                                | 60. Boris Averkiev, 2009-12                             |
| 29. Kiet Nguyen, 1994-96                                    | 61. Ruifang Li, 2009-10                                 |
| 30. Xavier Assfeld, 1994-96                                 | 62. John Alecu, 2009-12                                 |
| 31. Elena Laura Coitiño, 1995-97                            |   |
| 32. Maria Topaler, 1996-98                                  |   |

- |  |   |
|--|---|
| 63. Miho Isegawa, 2009-13 (joint with J. Gao, 2009-11) | 78. Guoliang Song, 2015-16                                  |
| 64. Anant Kulkarni, 2010-12                            | 79. Yinan Shu, 2016-present                                 |
| 65. Roberto Peverati, 2010–2012                        | 80. Xin-Ping Wu, 2016-19 (joint with L. Gagliardi, 2016-18) |
| 66. Xuefei Xu, 2010–2015                               | 81. Sijia Dong, 2017-19 (joint with L. Gagliardi, 2018-19)  |
| 67. Prasenjit Seal, 2011–2015                          | 82. Pragya Verma, 2017-18                                   |
| 68. Yuliya Paukku, 2011–2018                           | 83. Indrani Chaudhuri, 2018-20                              |
| 69. Rubén Meana-Pañeda, 2011-16                        | 84. Chen Zhou, 2018-21                                      |
| 70. Gbenga Oyedepo, 2011-13                            | 85. Dihua Wu, 2019-22                                       |
| 71. Zoltan Varga, 2012-15, 2016-22                     | 86. Jie Bao, 2021-24  |
| 72. Bo Wang, 2013-15                                   | 87. Farideh Badichi Akher, 2021-23                          |
| 73. Laura Fernandez, 2013-16                           | 88. Maryam Mansoori Kermani, 2022- 2024                     |
| 74. Max Makeev, 2014-15                                | 89. Qinghui Meng, 2023-present                              |
| 75. Wei Lin, 2014-15                                   | 90. Dayou Zhang, 2023-present                               |
| 76. Shuping Huang, 2014-16                             |   |
| 77. Wei-Guang Liu, 2014-17                             |   |

joint supervision with Christopher J. Cramer:

- |                                 |  |
|---------------------------------|--|
| 91. Joey W. Storer, 1993-94     | 97. Pablo Jaque, 2005-06   |
| 92. Tianhai (Tony) Zhu, 1996-98 | 98. Alek Marenich, 2006-16                                       |
| 93. Jiabo Li, 1997-99           | 99. Ryan Olson, 2006-07  |
| 94. Kevin Silverstein, 1998     | 100. Jingyun Ye, 2016-20 (also joint with L. Gagliardi, 2016-18) |
| 95. James Xidos, 1999-2001      |  |
| 96. Benjamin Lynch, 2003-05     |  |

joint supervision with Jiali Gao:

- |                            |                                      |
|----------------------------|--------------------------------------|
| 101. Tina Poulsen, 2001-02 | 103. S'moorthi Nachimuthu, 2010–2011 |
| 102. Jingzhi Pu, 2004-05   |                                      |

joint supervision with J. Ilja Siepmann:

104. Hannah Leverentz, 2012-13

joint supervision with Laura Gagliardi:

105. Andrew Sand, 2015-18  
 106. Kamal Sharkas, 2015-18  
 107. Bo Yang, 2016-19

### 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 Necoechea, 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
51. Siriluk Kanchanakungwankul, 2022
52. Jiaxin Ning, 2022
53. Dayou, Zhang, 2023
54. Suman Bhaumik, 2024

## 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 Pragya 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
- 22 Aiswarya M. Parameswaran, 2022

## 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 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 Zuebisch, 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 Goeppinger, 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, 2001-02
51. Amos Anderson, 2001-03
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 with C. Cramer
62. Hannah Leverentz, 2006-07
63. Jonathan Young, 2007
64. Alex Kozin, 2007
65. Robert Berscheid Jr. 2008-09
66. Di Wu, 2008-09
67. Raphael Ribiero 2009-10, joint with C. Cramer
68. Antonio de Oliviero-Filho, 2009
69. Sarah Kragt, 2009-10
70. Steve Jerome, 2009
71. Wendu Ding, 2009, joint w/ C. Cramer
72. Michelle Lenz, 2010
73. Duy P. Hua 2010
74. Gillian Shaw, 2011
75. Jeremy Tempkin, 2011
76. Abir Majundar, 2012-13, joint with C. Cramer
77. Helena Qi, 2012
78. Tiago Dominguez, 2012-13
79. Chad Hoyer, 2012, joint with L. Gagliardi
80. He Ma, 2014
81. Kelsey Parker, 2014, joint with L. Gagliardi
82. Siriluk Kanchanakungwankul, 2016-17

- |   |                             |
|---|-----------------------------|
| 83. Hirbod Heidari, 2017                          | 88. Lyuben Borislavov, 2019 |
| 84. Hung Vuong, 2018                              | 89. Shuhang Li, 2019-20     |
| 85. Kathleen Kidder, 2018                         | 90. Darya Snitovets, 2021   |
| 86. Kevin Huang, 2018-19                          | 91. Bhavnesh Jangid, 2022   |
| 87. Erica Mitchell, 2019, joint with L. Gagliardi | 92. Shaoting Zhang, 2023-24 |

**Outside examiner, Ph.D. Theses:**

- John Scott Carley, University of Waterloo (Canada), 1978  
 Margot Mandy, University of Toronto (Canada), 1991  
 Justin Villard, Ecole Polytechnique Fédérale de Lausanne, 2023

**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, 2002-03 (sabbatical), 2004, 2005  
 Yaakov Shima, 1986  
 Yici Zhang, 1987  
 Yan Sun, 1987  
 Prof. Antonio J. C. Varandas, 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, 2023, 2024  
 Prof. Piotr Paneth, 2000-01 (sabbatical)  
 Prof. Przemek Staszewski, 2002-03, 2004, 2005  
 Prof. Joseph Brom, 2002-03 (sabbatical)  
 John Keith, 2002

Agnieszka Dybala-Defratyka, 2002  
 Iva Tatic, 2002  
 Prof. Larry Pratt, 2003, 2004  
 Prof. Keith Kuwata, 2003-04 (sabbatical)  
 Luis Campos, 2003  
 Prof. Clayton Spencer, 2004-05  
 Nuria Gonzalez, 2004, 2005  
 Javier Ruiz Pernia, 2004, 2005  
 Jaiyun Pang, 2004-05  
 Prof. Masato Nakamura, 2005  
 Shivangi Nangia, 2005  
 Prof. Sonia Ilieva, 2005-06 (Fulbright Fellow)  
 Michal Rostkowski, 2005  
 Prof. Jonathan Smith, 2006-07 (sabbatical)  
 Neil Young, 2006  
 Yihan Shao, 2006-07  
 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, 2009-10  
 Varinia Bernales, 2011-12  
 Amrit Jalan, 2012  
 Wenjing Zheng, 2012-14  
 Pattrawan Sripa, 2014  
 Prof. Xiao He, 2014, 2015  
 Xiaoyu Li, 2015-16  
 Prof. Xin Zhang, 2015-16  
 Prof. Bo Long, 2015-16  
 Andrey Pershin, 2016  
 Prof. Xuefei Xu, 2017  
 Lili Xing, 2016-17  
 Wanqiao Zhang, 2016-17  
 Linyao Zhang, 2017-19  
 Prof. Yan Zhao, 2018  
 Lu G. Gao, 2018-19  
 Junjun Wu, 2019  
 Shuhang Li, 2019  
 Xu Cai, 2019-20  
 Xiaozhe Fan, 2019-20  
 Rui Ming Zhang, 2019-20  
 Yao-Yuan (John) Chuang, 2022  
 Bhavnesh Jangid, 2022  
 Shaoting Zhang, 2023-24

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### **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

