

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-present

Graduate Minor Program in Nanoparticle Science and Engineering

Charter Member of Graduate Faculty, beginning 2002

Battelle Memorial Institute: Columbus, Ohio, Visiting Fellow, 1973.

Joint Institute for Laboratory Astrophysics, Boulder, Colorado: Visiting Fellow, 1975-76.

Academies

American Academy of Arts and Sciences, 2015

International Academy of Quantum Molecular Science, 2006

National Academy of Sciences, 2009

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
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, 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 R. Herschbach Award for Research in Collision Dynamics, 2009

The award 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

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.”

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, June 8, 2017

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.

Research

Professor Truhlar’s research is in theoretical and computational chemistry, with emphases on kinetics, dynamics, solvation, electronic structure, and thermochemistry. Special emphases:

- the study of photoactivated processes, for which his work includes excitation energies, potential energy surfaces and their couplings, and multi-state dynamics
- the incorporation of quantum effects in dynamics, including tunneling, vibrational quantization and anharmonicity, 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, nanodusty plasmas, surface science, and enzyme kinetics
- 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
- transition metal chemistry, with a special emphasis on catalysis
- computational thermochemistry, including free energies of complex species in the gas phase and solution, solvation free energies, and electrochemistry

- new methods for path integral calculations in quantum mechanical statistical mechanics
- lithium-ion battery development: structure, electromotive force, capacity, and transport

Bibliography

1142 journal articles, 86 book chapters, 14 books edited.

Bibliography: <http://comp.chem.umn.edu/Truhlar/>

Citation Statistics

Statistics from Google Scholar, August 5, 2017:

Number of citations: 129,355. h-index: 155. i10 index: 1099.

56 articles with 400 or more citations.

<https://scholar.google.com/citations?user=1gaf87YAAAAJ&hl=en&cstart=40&pagesize=20>

Statistics from ISI Web of Science, June 17, 2017:

Number of citations: 100,494 in 43,211 articles. h-index: 139.

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)

Listed by Thomson Reuters in *The World's Most Influential Scientific Minds: 2014*

“This list of top researchers around the globe have earned their distinction by publishing the highest number of articles that rank among those most frequently cited by fellow researchers.... Highly cited papers rank in the top 1% by citations for their field and year of publication.... These highly cited researchers were determined by analyzing at citation data over the last 11 years to identify those who published the highest- impact work (2002–2012 and 2012–2013).”

<http://thomsonreuters.com/en/articles/2014/worlds-most-influential-scientific-minds-2014.html>

<http://sciencewatch.com/sites/sw/files/sw-article/media/worlds-most-influential-scientific-minds-2014.pdf>

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 21st most highly cited paper in the history of the journal, out of 154,000 papers published and is the only article published in the last twelve years that is included in the announced list of the top 25.



Highly Cited Researcher

2001-14

<http://hcr.stateofinnovation.thomsonreuters.com/page/archives>

2015

<http://highlycited.com/>

2016

http://hcr.stateofinnovation.thomsonreuters.com/?utm_campaign=14406-2016%20HCR%20emails%20V1-%20Sep%206-31113&utm_medium=email&utm_source=Eloqua

Synergistic Activities

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, years confidential, including chair
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 committee, year confidential

Other organization of conferences and symposia, organizer or co-organizer:

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

American Conf. on Theoretical Chemistry, vice chair 1984, chair (elected 1981) 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 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-present.

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

Editor or co-editor, fourteen books.

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.

Editorial Boards:

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

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)
Chemical Physics, Advisory Ed. Board, 2005-present.
Molecules, Section Ed., 2016

Recent reviewer recognition:

2014 Outstanding Referee of the *Physical Review* and *Physical Review Letters*

Recognized by the American Physical Society as one of 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".

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

Teaching

Graduate courses taught:

- Chemical 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 neuroscience (guest lecturer)
- Computational chemistry (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: 82 (67 publications with 47 different undergraduate coauthors)

Graduate: 57 completed Ph.D. or both Ph. D. and M. S., 12 completed with M. S., 7 currently working toward Ph. D.

Postdoctoral: 98

Honors awarded to research students I have 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)
- 1992 Yi-Ping Liu: John Overend Award for Graduate Research in Physical Chemistry
- 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
- 1993 Stephen Mielke: John Wertz Award for Outstanding Graduate Research in Chemical Physics
- 1994 Wei-Ping Hu: John Overend Award for Graduate Research in Physical Chemistry
- 1997 Yao-Yuan Chuang: John Wertz Award for Outstanding Graduate Research in Chemical Physics
- 1999 Michael D. Hack: John Overend Award for Graduate Research in Physical Chemistry
- 2001 Jason Thompson: Midwest Theoretical Chemistry Conference Dirac Award for Outstanding Graduate Research in Theoretical Chemistry
- 2001 Ahren Jasper: John Overend Award for Graduate Research in Physical Chemistry
- 2002 Amos Anderson: Thomas DuBruil Undergraduate Research Award, University of Minnesota
- 2003 Jason Thompson: Chemical Computing Group Excellence Award for National ACS Meeting
- 2003 Amos Anderson: 2003 Peter Auzins Memorial Scholarship and Senior Prize for outstanding achievement in undergraduate research
- 2003 Jingzhi Pu and Jason Thompson: co-recipients of the John Overend Award for Graduate Research in Physical Chemistry
- 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"
- 2006 Erin Dahlke: John Overend Award for Graduate Research in Physical Chemistry
- 2007 Nathan Schultz: University of Minnesota Graduate School's "Best Dissertation Award, Physical Sciences and Engineering" for his Ph. D. thesis entitled "Computational Nanoscience"
- 2010 Bo Wang: John Overend Award for Graduate Research in Physical Chemistry

- 2011 Hannah Leverentz: John Overend Award for Graduate Research in Physical Chemistry
- 2012 Sijie Luo: Beaker and Bunsen Award, University of Minnesota 2012 Graduate Student Research Symposium
- 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”
- 2015 Junwei (Lucas) Bao: best poster prize at the 15th International Congress of Quantum Chemistry
- 2016 Shaohong Li: John Overend Award for Graduate Research in Physical Chemistry
- 2016 Junwei (Lucas) Bao: Beaker and Bunsen award winner at the 15th annual Graduate Student Research Symposium
- 2017 Junwei (Lucas) Bao: John Overend Award for Graduate Research in Physical Chemistry

Recent fellowships awarded to students in my group

- 2011 Bo Wang: 2011-2012 Doctoral Dissertation Fellowship
- 2013 Pragma Verma: 2013-2014 Phillips 66 Excellence Fellowship
- 2013 Haoyu Yu: 2013-14 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

Research support

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
- Petroleum Research Fund of the American Chemical Society
- Minnesota Dept. of Employment and Economic Development

Foundation:

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

Other computational resources:

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