

Curriculum Vitae of Donald G. Truhlar

Born: Chicago, February 27, 1944

Education

Our Lady of Holy Mount grammar school, Cicero, Illinois, graduated 1958

St. Mel High School, Chicago, graduated 1961

St. Mary's College, Winona, Minnesota, B.A., summa cum laude, 1965, major: chemistry, minor: mathematics

California Institute of Technology, Pasadena, Ph.D., 1970, major: chemistry

Professional Experience, University of Minnesota

Department of Chemistry

Graduate Faculty, 1969–present

Assistant Professor, 1969–72

Associate Professor, 1972–76

Professor, 1976–present

Director of Graduate Studies, 1986–88

George Taylor Institute of Technology Professor, 1993–98

Institute of Technology Distinguished Professor, 1998–present

Lloyd H. Reyerson Professor, 2002–present

Chemical Physics Program

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–present

Graduate Program in Scientific Computation

Founding Director of Graduate Studies, 1990–96, 2002

Graduate Faculty, 1990–present

Graduate Minor program in Nanoparticle Science and Engineering

Graduate Faculty, 2002–present

Other

Argonne National Laboratory, research in Myran Sauer lab, 1965

Los Alamos National Laboratory, consultant, 1972–1992. Host: Normand C. Blais

Battelle Memorial Institute, Columbus, Ohio, Visiting Fellow, 1973. Hosts: Bill Kern and Shi Shavitt

Joint Institute for Laboratory Astrophysics of the University of Colorado and the National Bureau of Standards, Boulder, Colorado, Visiting Fellow, 1975–76. Hosts: Bill Reinhardt and Carl Lineberger

Professional Honors

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

“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”

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

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”

Lise Meitner Lectureship Award for the year 2006

“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”

American Chemical Society Peter Debye Award in Physical Chemistry, 2006

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

Selected Major Lectures

David Bates Honorary Symposium, 1983

DuPont Distinguished Lecturer, University of Indiana, 1990

Michael Kasha Honorary Symposium, 1991

Arthur William Davidson Lectureship, University of Kansas, 1991

Max Bodenstein Centennial Symposium, 1995

Distinguished Lectureship, Louisiana State University, 1996

Faraday Discussion Chemical Reaction Theory, summarizing lecturer, 1998

American Physical Society Centennial Lecturer, 1999

Frontiers In Chemical Research Lectureship, Texas A & M University, 2003

Mulliken Lectureship, University of Georgia, 2003

Svante Arrhenius Centennial Symposium, 2003

Faraday Discussion Nonadiabatic Effects in Chemical Dynamics, Introductory Lecturer, 2004
 Kilpatrick Lecturer, Illinois Institute of Technology, 2004
 Nicholas Handy Honorary Conference, 2004
 Jacopo Tomasi Honorary Symposium, 2004
 John Pople Memorial Symposium, 2005
 Washburn Lecturer, University of Nebraska, 2005
 Neckers Lecturer, Southern Illinois University, 2006

Editorships and Editorial Boards

Journal of Chemical Physics, Associate Editor, 1978–80
Chemical Physics Letters, Advisory Editor, 1982–present
Journal of the American Chemical Society, Associate Editor, 1984–2002, Board of Editors, 2003–present
Theoretical Chemistry Accounts (Theoretica Chimica Acta), Editor, 1985–98, Associate Editor, 1998–2001, Chief Advisory Editor, 2002–present
Journal of Physical Chemistry, Advisory Board, 1985–87
Computer Physics Communications, Editor, 1986–present
Reports in Molecular Theory, Editorial Board, 1989–90
Understanding Chemical Reactivity, Series Editor, 1990–92, Editorial Advisory Board, 1987–90, 1992–99
Topics in Physical Chemistry, Series Editor, 1992–99
IEEE Computational Science & Engineering, Area Editor for Computational Chemistry, 1993–98
Advances in Chemical Physics, Editorial Board, 1993–present
International Journal of Modern Physics C, Editorial Board, 1994–2005
International Journal of Quantum Chemistry, Advisory Editorial Board, 1996–2000
Computing in Science and Engineering, Applications Editor, 1999–2005
Journal of Computational Methods in Sciences and Engineering, Editorial Board, 2001
PhysChemComm, Advisory Editorial Board, 2001–03
Central European Journal of Chemistry, Editorial Board, 2002–present
Journal of Chemical Theory and Computation, Advisory Board, 2004–present
Chemical Physics, Advisory Editorial Board, 2005–09
 Editor or co-editor, thirteen books

Professional Society Offices

Secretary, Subdivision of Theoretical Chemistry, American Chemical Society, 1981–89
 Councilor, American Chemical Society, elected by Physical Chemistry Division 1984, served 1985–87

Major Conference Chairmanships

Conference on the Dynamics of Molecular Collisions, elected 1981, chairman 1985
 American Conference on Theoretical Chemistry, elected 1981, chairman 1987
 International Symposium on Computational Chemical Dynamics, organizer, 1994

More than 20 other national and international conferences, symposia, and workshops

Selected National Committee Service

American Chemical Society: Physical Chemistry Executive Committee, Task Force on Publication in Molecular Modeling, other committees, 1980–89, 1991–95, 1999–2004
 American Physical Society: committees of Topical Group on Few-Body Systems and Multiparticle Dynamics and Division of Computational Physics, Working Group on Physics and Astronomy Classification Scheme, 1988–90, 2000–02, 2005–06
 Council for International Exchange of Scholars: Advisory Screening Committee in Chemistry (selection of Fulbright Fellows), 1977–80
 International Union of Pure and Applied Chemistry: Commission on Physical Organic Chemistry, 1997–8
 National Research Council: Committee on Kinetics of Chemical Reactions, Panel for Chemical Physics, and Nominating Committee, 1977–80, 1983, 1986–88
 U.S. Department of Energy: Roadmap Committee, 1998

Major Research Support

National Science Foundation, 1971–present
 U.S. Department of Energy, Office of Basic Energy Sciences, 1979–present
 National Aeronautics and Space Administration, 1978–80, 1987–95
 Department of Defense, 1989–96, 2001–present
 Also: Control Data Corporation, Cray Research, Eastman Kodak Corporation, Minnesota Dept. of Employment and Economic Development, National Institute of Standards and Technology, Petroleum Research Fund of the American Chemical Society, Phillips Petroleum
 Computational resource grants: Army High-Performance Computing Research Center, Maui High Performance Computing Center, National Center for Atmospheric Research, National Resource for Computation in Chemistry, NSF supercomputer program, The William R. Wiley Environmental Molecular Sciences Laboratory
 Training grants: NSF IGERT, NSF REU, NSF RSEC, NIH

Teaching

Chemical dynamics, general principles of chemistry, quantum chemistry, quantum mechanics, reaction kinetics, statistical mechanics, supercomputer research, thermodynamics, topics in physical chemistry

Distributed Computer Programs

ABCRATE, AMM, AMSOL, AMSOLRATE, CGPLUS, CRATE, DCS, DGSOL, DIRDYVTST, EHT, FDBVM, GAMESSPLUS, GAMESSPLUSRATE, GAUSSRATE, HONDOPLUS, KAPPAS, MC-TINKER, MC-TINKER-ATE, MLGAUSS, MNN, MOPACmn, MORATE, MORSEX, MULTILEVEL, MULTILEVELRATE, NETI, NETIX, OMNISOL, POLYRATE, QMMM, RMPROP, SMX-GAUSS, TB, VIBCI, ZINDO99.1