Curriculum Vitae of Thom Dunning, Jr.

Education

University of Missouri−Rolla, B.S. 1965. Major: chemistry. Minors: physics, mathematics

California Institute of Technology, Ph.D., 1970. Major: chemistry (Advisor: B. Vincent McKoy)

Research Fellow, Battelle Memorial Institute, 1970−71 (Advisor: Russell M. Pitzer)

Research Fellow and Instructor, California Institute of Technology, 1971−73 (Advisor: William A. Goddard III)

Professional Experience

Director, National Center for Supercomputing Applications, University of Illinois at Urbana−Champaign, 2004−present

Distinguished Chair for Research Excellence, Department of Chemistry, University of Illinois at Urbana−Champaign, 2004−present

Director (Founding), Joint Institute for Computational Sciences, University of Tennessee−Oak Ridge National Laboratory, 2002−04

Distinguished Professor, Department of Chemistry, University of Tennessee, 2002−04

Distinguished Scientist, Computing and Computational Sciences, Oak Ridge National Laboratory, 2002−04

Vice President, High Performance Computing and Communications, MCNC (Research Triangle Park), 2001−02

Professor, Department of Chemistry, University of North Carolina at Chapel Hill, 2001−04

Assistant Director for Scientific Simulation, Office of Science, U.S. Department of Energy, 1999−2001 (on leave from Pacific Northwest National Laboratory)

Battelle Fellow, Pacific Northwest National Laboratory, 1997−2001.

Manager of Fundamental Science, Pacific Northwest National Laboratory, 1997−99

Director, Environmental and Molecular Sciences Laboratory, Pacific Northwest National Laboratory, 1994−97

Associate Director, Theory, Modeling & Simulation, Environmental and Molecular Sciences Laboratory, Pacific Northwest National Laboratory, 1989−94

Associate Director, Computer & Information Science, Environmental and Molecular Sciences Laboratory, Pacific Northwest National Laboratory, 1992−94

Group Leader, Theoretical & Computational Chemistry Group, Argonne National Laboratory, 1978−89

Staff Member, Laser Theory Group, Physical Chemistry Group, Los Alamos National Laboratory, 1973−78

Other Appointments

Visiting Professor, Department of Chemistry, University of Colorado, 1989

Affiliate Professor, Department of Chemistry, University of Washington, 1990−2001

Adjunct Professor, Department of Chemistry, Washington State University, 1990−2001

Winslow Fellow, Department of Chemistry, University of Melbourne (Australia), 1996

Visiting Distinguished Scientist, Computing and Computational Sciences, Oak Ridge National Laboratory, 2004−present

Professional Honors

Woodrow Wilson Foundation Graduate Fellowship, 1965−66

National Science Foundation Graduate Fellowship, 1966−69

Fellow, American Physical Society, 1992

Fellow, American Association for the Advancement of Science, 1992

E. O. Lawrence Award in Chemistry, U.S. Department of Energy, 1996. Citation: For seminal contributions to the advancement of molecular electronic structure theory and computations; for applications to fundamental problems in chemical laser development, combustion chemistry, and environmental chemistry; and for leadership in the utilization of high performance computing for solving chemical problems.

Award for Excellence in Technology Transfer, Federal Laboratory Consortium for Technology Transfer, 2000. Citation: "The Molecular Science Software Suite (MS3) is the first general purpose software that provides access to the high-performance, massively parallel computers for chemists on a broad range of applications."

Distinguished Associate Award, U.S. Department of Energy, 2001. Citation: "In recognition of over 27 years of exemplary scientific research, management, and leadership and outstanding contributions in chemical, molecular, and computational sciences for the Department. In particular, your leadership in the Chemical Dynamics Program, the Environmental Molecular Sciences Laboratory, and the Scientific Discovery through Advanced Computing Program have made a significant impact on the Department of Energy and the Scientific Community."

Professional Degree in Chemistry, University of Missouri−Rolla, 2005

Editorship and Editorial Boards

Editor, *Advances in Molecular Electronic Structure*, JAI Press, Inc., 1987−95

Topical Editor, *Computer Physics Communications*, 1989−97

Editorial Board, *Journal of Chemical Physics*, 1998−2001

Major Committee Assignments

Member, Advisory Board, Foundation for Chemical Research, Department of Chemistry, University of Missouri−Rolla, 1984−94

Member, Energy Sciences Network Steering Committee, Office of Scientific Computing, U.S. Department of Energy, 1986−89

Chairman, Tank Waste Science Panel, Pacific Northwest National Laboratory, 1990−92.

Member, Policy Board, Concurrent Supercomputing Consortium, California Institute of Technology, 1990−96

Member, Advisory Committee for Chemistry, Chemistry Division, National Science Foundation, 1991−93

Member, Advisory Committee, Combustion Research Facility, Sandia National Laboratories−Livermore, 1995−99

Member, Advisory Council, Washington State University−TriCities, 1995−98

Member, Council on Chemical Sciences, Chemical Sciences Division, Office of Energy Science, U.S. Department of Energy, 1996−99

10.1021/jp077139h
Published on Web 11/01/2007

Vice Chairman, Chemical Sciences Roundtable, Board on Chemical Science and Technology, National Research Council, 1996−99

Member, Science and Technology Advisory Committee, Brookhaven National Laboratory, 1997−99

Chair, Scientific Advisory Board, Institute of High Performance Computing (Singapore) 2006−present

Conferences and Symposia Chairmanships

DOE/OBES Combustion Research Meeting, Argonne National Laboratory, 1980

DOE/OBES Combustion Research Meeting, Interlaken Conference Center, 1985

Symposium on "Theory and Simulation in Chemistry: The Impact of Mini-supercomputers and Supercomputers," 193rd National Meeting of the American Chemical Society, Denver, Colorado, 1987 (co-organized with R. L. Shepard and L. Anacker)

DOE/OBES Combustion Research Meeting, Interlaken Conference Center, 1988

13th Annual West Coast Theoretical Chemistry Conference, Pacific Northwest National Laboratory, Richland, Washington, 1992.

"Workshop on High Performance Computing in Chemistry," National Institutes of Health, Bethesda, Maryland, 1993 (co-organized with R. A. Kendall, W. P. Reinhardt, and B. Brooks)

Symposium on "Physical Chemistry and the Environment," 206th National Meeting of the American Chemical Society, Chicago, Illinois, 1993 (co-organized with B. C. Garrett)

Workshop on "Assessing the Value of Research in Chemical Science and Technology," National Academy of Sciences, 1997

Workshop on "Impact of Advances in Computing and Communication on Chemical Science and Technology," National Academy of Sciences, 1998

"Computational Chemistry in the 21st Century: Methods and Applications" for the International Conference for Computational Science, Melbourne, Australia, 2003 (with R. J. Harrison, ORNL/UT; L. Radom, University of Sydney; and A. Rendell, Australian National University)

First Fall Creek Falls Workshop on Computational Science and Engineering, Fall Creek Falls State Park and Resort, Pikeville, Tennessee, 2003

Teaching

Nature of the chemical bond (with W. A. Goddard, III), theory of molecular structure and energetics, electronic structure of molecules

Major Research Support

National Nuclear Security Administration, U.S. Department of Energy, 1973−78

Office of Science, U.S. Department of Energy, 1978−2001

National Science Foundation, 2002−present