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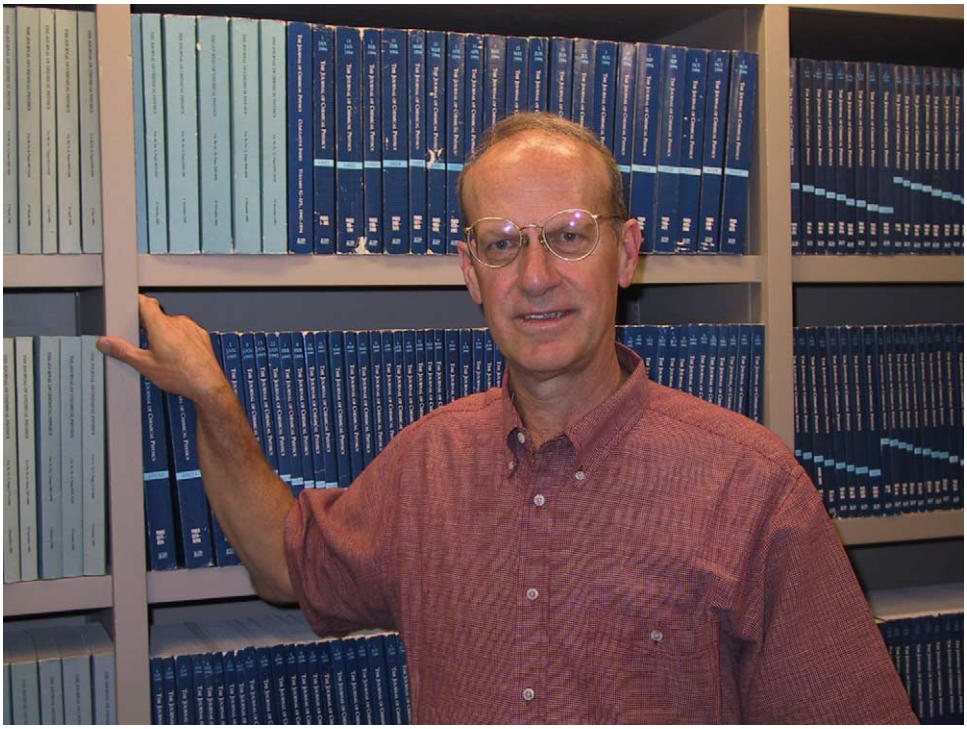
Tribute

A celebration of the scientific and personal contributions of William L. Hase



Bill was born in 1945 in Washington, Missouri. He attended Mexico Senior High School in Mexico, Missouri where he particularly enjoyed mathematics and chemistry, and was strongly influenced by his chemistry teacher George Craddock. He began his professional education at the University of Missouri, Columbia, Missouri. There he started out as a chemical engineering major, but switched to chemistry to avoid the required applied chemical engineering labs. At Missouri, Bill was inspired by Lloyd Thomas, a great thermodynamics professor.

Bill decided to pursue his Ph.D. studies out west and received his Ph.D. in chemistry, with minors in physics and mathematics in only 3 years of graduate work at New Mexico State University in Las Cruces, New Mexico. It may come as a surprise to many of you that his Ph.D. research area was actually experimental physical chemistry. Under the guidance of his Ph.D. mentor Professor John W. Simons, he studied experimental gas phase kinetics with applications to the determination of the methylene singlet-triplet gap and the unimolecular decomposition of vibrationally excited alkane and alkylsilane molecules prepared by chemical activation. After completing his Ph.D., Bill stayed on for another year at New Mexico State University to run his mentor's research group while Simons was on sabbatical in England. Bill's aversion to experimental work became evident in his choice of postdoctoral research area. He began his career as a computational chemist by working with Professor Don Bunker at the University of California, Irvine. Under Bunker's direction, Bill studied RRKM and non-RRKM unimolecular kinetics and the effects of exit-channel coupling on the unimolecular

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decomposition of a variety of small molecules. He credits Bunker with inspiring and convincing him to embark on an academic career. In 1973, he joined the Chemistry Department at Wayne State University as an assistant professor of chemistry and quickly rose through the ranks. He was promoted to Associate Professor in 1978, Full Professor in 1981, elected to lifetime membership in the Academy of Scholars in 1994, and was recognized as a Distinguished Professor in 1997.

At Wayne State, Bill started his renowned work on molecular and chemical reaction dynamics. He fondly remembers the assistance given to him by fellow Wayne State University faculty member Larry Kevan, an outstanding Electron Spin Resonance (ESR) spectroscopist. (Kevan later moved to the University of Houston and passed away in 2003.) Kevan graciously permitted his own postdoc to work with Bill, helping to jump start his research program. Over the years, Bill's research group has developed theoretical methods for the computer simulation of chemical reaction dynamics. He remembers that his first computational chemistry classical trajectory program was written in assembly language and ran on a DEC PDP-10 (an early multi-user mainframe computer). Since that time, Bill's group and computers have come a long way; they are now able to simulate ab initio chemical reaction dynamics "on the fly" using VENUS (the Hase group's most recent general chemical dynamics computer program) on a desktop workstation. As every great computational (and experimental) chemist recognizes, theoretical models are very useful for the proper interpretation of experimental data, but are most insightful when then can be used in a predictive fashion. Bill has taken this creed to heart in all of his research endeavors, by applying the computation methods his group has developed to a wide variety of chemical systems. These range from gas-phase unimolecular and bimolecular reactions, to liquids, collisions of gas phase ions with surfaces, and structure, adhesion, and friction of interfaces.

Some of his more important work includes studies of gas-phase S_N2 reactions in which the underlying atomic level mechanisms are elucidated, and his simulations-based research on RRKM theory in which he extended the seminal work of Stanford's John Brauman. Bill is also particularly proud of his group's contributions to the understanding of intramolecular dynamics and molecular motion leading to non-RRKM behavior as described in the *Journal of Chemical Physics*, 73 (1980) 3779–3790. His group has made major contributions to the understanding of energy deposition and fragmentation processes involved in collision-induced and surface-induced dissociation. Our understanding of the structure, energetics, and dynamics of interfaces, including the characterization of friction and adhesion at heterogeneous boundaries, has been improved by insightful work from the Hase group.

Bill has published over 200 peer-reviewed research papers and seven review articles. He has also authored two books and 23 book chapters. I'm sure every reader, either as a student or professor, has used the book that Bill coauthored with J.I. Steinfeld and J.S. Francisco entitled, "Reaction Kinetics and Dynamics", currently in its second edition. Personally I have used this book as a student, a professor, and as a researcher and have found it to be a great resource (even though they keep me on my toes, I do hope that he eliminates more of the typos in the third edition). Bill also coauthored "Unimolecular Reaction Dynamics—Theory and Experiments" with Professor Tom Baer, another useful research and teaching resource. Bill has had an important influence on many experimental groups because of the clarity of his papers and his presentations. No one who reads his paper on "Variational Unimolecular Rate Theory", *Acc. Chem. Res*. 16 (1984) 258–265, can fail to understand this important theory. Tom Baer said that he learned more about unimolecular reactions from Bill than anyone else because he has such a broad and balanced understanding of the field, and a unique ability to communicate it (perhaps a result of his early training as an experimentalist).

Over the years, Bill has contributed to the teaching and curriculum development at both the undergraduate and graduate levels teaching courses in Chemistry for Liberal Arts and Humanities, General Chemistry I and II, Biological Physical Chemistry, and Physical Chemistry I and II for undergraduates, and Statistical Thermodynamics, Chemical Kinetics, Molecular Dynamics and Monte Carlo Simulations, Molecular Reaction Dynamics, and Scientific, Engineering, and Medical Applications of Modeling and Simulation for graduate students. In 1997, Bill was recognized for his contributions to teaching with a Wayne State University College of Science Excellence in Teaching Award. He was also largely responsible for establishing the NSF-IGERT funded Institute for Scientific Computing at Wayne State University, which trains graduate students from several departments in interdisciplinary high performance computing applications.

Through the years, Bill has had the opportunity to work with a large number of talented graduate students and postdoctoral fellows as evidenced by his many contributions to chemical reaction dynamics. He has also been very fortunate to work with a number of outstanding undergraduate students, the most well known being Tamar Schlick, a professor of chemistry, mathematics, and computer science at New York University, who credits Bill with making her into a research scientist.

Bill's accomplishments have been recognized throughout the years in several ways. He has received an Outstanding Performance Award from the National Science Foundation. He is a Fellow of the American Physical Society, appointed for his "extensive contributions to the theory of unimolecular and intramolecular dynamics, variational transition state theory, and the classical trajectory approach for studying chemical reaction dynamics". He is also a Fellow of the American Association for the Advancement of Science (AAAS). Further, he has served the scientific community well, for instance, as chairman of the Theoretical Chemistry Subdivision of the ACS Division of Physical Chemistry.

I remember first meeting Bill when he came to Caltech to give a Chemical Physics seminar during my postdoctoral

work with Jack Beauchamp. His computer animations of chemical reaction dynamics really excited us and inspired our attempts to simulate collisional activation of biological molecules. Somewhat naïve at the time, I had never heard of Wayne State University, but after the seminar, I realized that a lot of exciting research was being carried out there. Therefore, when the opportunity for me to join the faculty at Wayne State arose a few years later, I was very excited about this position and the opportunity to have Bill as a fellow colleague. In 2004, Bill decided to return to the west and moved to the Chemistry Department at Texas Tech University where he is the Robert A. Welch Professor of Chemistry. Although I was very disappointed at losing such a valuable colleague, this change has created a new avenue for collaboration between Bill and me. We now share a graduate student who is pursuing simulations of the surface-induced dissociation of protonated peptides on fluorinated self-assembled monolayer (F-SAM) surfaces.

It should be obvious that a 60th birthday is an opportunity to recognize and thank a deserving scientist, colleague, and friend. With his re-birth as a Texan and the opportunities provided for him by Texas Tech, Bill's enthusiasm for science and life is as high as ever. We can look forward to many new and exciting discoveries in chemical reaction dynamics from Bill and his research group. Bill, may your coming years be filled with insight, achievement, and enjoyment.

William Louis Hase: Curriculum Vitae

Education

1967	B.S., Chemistry, University of Missouri, Columbia, Missouri
1970	Ph.D., Chemistry, New Mexico State University, Las Cruces New Mexico
1970–1971	Postdoctoral research, New Mexico State University, Las Cruces, New Mexico
1971–1973	Postdoctoral research, University of California, Irvine, California
1981	Sabbatical research, University of California, Berkeley, California
1991	Sabbatical research, University of Colorado, Boulder, Colorado
1995	Sabbatical research, Ford Scientific Research Laboratories, Dearborn, Michigan
1999	Sabbatical research, University of Utah, Salt Lake City, Utah

Professional Experience

1973–1978	Assistant Professor of Chemistry, Wayne State University
1978	Visiting Professor of Chemistry, University of California, Irvine, California
1978–1981	Associate Professor of Chemistry, Wayne State University
1981–1997	Professor of Chemistry, Wayne State University
1997–2003	Distinguished Professor of Chemistry, Wayne State University
1999–2003	Director, Institute for Scientific Computing, Wayne State University
2001–2003	Chair, Department of Computer Science, Wayne State University
2004	Robert A. Welch Professor of Chemistry, Texas Tech University

Professional Societies and Association Memberships

American Chemical Society

American Physical Society

American Association for the Advancement of Science

Sigma Xi (Chemistry Honorary)

Sigma Pi Sigma (Physics Honorary)

Fellowships and Honors

1963	NROTC Undergraduate Scholarship (University of Missouri)
1963–1965	University of Missouri Curators Scholarship
1968–1970	NDEA Predoctoral Fellowship (New Mexico State University)
1985	Outstanding Performance Award, National Science Foundation
1987–1988	One of 100 Outstanding Graduates of the College of Arts and Science during New Mexico State University's Centennial Year
1991	Fellow of the American Physical Society
1994	Academy of Scholars, Wayne State University
1994	Visiting Fellowship from the Sonderforschungsbereich "Molekulare Mechanismen Unimolekularer Prozesse", Max-Planck-Institut für Strömungsforschung Göttingen, Germany
1995–1997	Board of Governors Distinguished Faculty Fellowship, Wayne State University
1996	Leader in Chemistry in the College of Arts and Science, University of Missouri, Columbia, Missouri
1997	College of Science Excellence in Teaching Award, Wayne State University

1997	Fellow of the American Association for the Advancement of Science
1997	Academy of Scholars, Wayne State University

Professionally Related Service and Activities

Editor of *Advances in Classical Trajectory Methods*, published by JAI Press Inc.

Member of the *Southern Brazilian Journal of Chemistry* Editorial Board 1993-

Member of the *Journal of Physical Chemistry* Advisory Board, 1995–2000

Reviewer for Granting Agencies: National Science Foundation, Department of Defense, Department of Energy, Petroleum Research Fund, Research Corporation, Nato Advanced Study Institute, United-States Israel Binational Science Foundation, NSERC-Canada, Swiss National Science Foundation.

Reviewer for Research Publications: Journal of Chemical Physics, Journal of Physical Chemistry, Chemical Physics Letters, Molecular Physics, Chemical Physics, Journal of the American Chemical Society, International Journal of Chemical Kinetics, Accounts of Chemical Research, International Journal of Quantum Chemistry, Astrophysical Journal Letters, Inorganic Chemistry, Physical Review, Journal of the Optical Society of America B, Journal of Computational Chemistry, Physics Letters A, Computers and Chemistry, Journal of Organic Chemistry, Science, Journal of Chemical Education, Physical Chemistry Chemical Physics, Journal of the American Society for Mass Spectrometry, Chemistry-A European Journal. Journal of Physical Organic Chemistry, Tribology Letters, International Journal of Mass Spectrometry, Chemistry of Materials, Angewandte Chemie, Chemical Physics Physical Chemistry, Organic Letters, Chemical Reviews, Physical Review Letters, Journal of computational and Theoretical Chemistry, International Review of Physical Chemistry, New Journal of Chemistry

Assistant Director for the *3rd Winter Course in Gas Kinetics*, Lake Arrowhead California, 1973.

Program Officer for Theoretical Chemical Physics, National Science Foundation, Washington, D.C., 1983–84.

National Science Foundation representative at the workshop on *Future Directions for Supercomputer Use in Chemistry*, 1984.

Member of the Charter Committee to Support the Chemistry Department, University of Missouri, Columbia, 1985–1988.

Chairman of the Nominating Committee for the American Chemical Society Theoretical Chemistry Subdivision, 1985.

Participant in a *National Science Foundation Workshop on Theoretical Chemistry*, 1986.

Member of the National Science Foundation Site Visit Team, Minnesota Supercomputer Center, 1986.

Member of NSERC Site Visit Team, TRIUMF, Vancouver, British Columbia, Canada, January 16, 1991.

Member of U.S. Department of Energy Panel to Review Combustion Related Research Programs in Quantum Chemistry and Dynamics, 1992.

Member of AFOSR Chemical Sciences Review Panel, National Academy of Sciences, Washington, DC, 1993.

Member of Scientific Organizing Committee for the First Electronic Computational Chemistry Conference, 1994.

Participant in an AFOSR Theory-Synthesis Workshop, 1995.

Member of the Panel for Review of Programs in Chemical Physics at the Environmental and Molecular Sciences Laboratory, Pacific Northwest Laboratories, Richland, Washington, 1996.

President and Member of Board of Directors of Mesilla Chemistry Workshop Inc. (1997–present)

Participant in Workshop for DOE's Strategic Simulation Initiative: *The Combustion Simulation and Modeling Initiative*, Washington, DC, 1998.

Presentation of the Interdisciplinary Program on *Scientific Computing* to the College of Science Advisory Board, 1998.

Member of the Panel for Review of Gas-Phase Chemical Dynamics Program at Argonne National Laboratory, 1998.

Guest Editor (with Wolfram Koch) of Volume 201, 2000 of the *International Journal of Mass Spectrometry*. A special issue addressing *Theoretical/Computational Studies of Ionic Systems.*

Computational Chemical Dynamics Review, Office of Naval Research, Arlington, Virginia, 2001.

Participant in the University of North Carolina and North Carolina Supercomputing Center Workshop on *Computational Modeling in Science and Engineering Education*, 2002.

Vice-Chair, 7th Winter Gordon Conference on *Gaseous Ions: Structure, Energetics and Reactions*, March 2–7, 2003, Ventura, CA.

Guest Editor (with Gustavo Scuseria) of Volume 5, 2003 of *Computing in Science and Engineering*. A special issue addressing *Computational Chemistry.*

Chair, 8th Winter Gordon Conference on *Gaseous Ions: Structure, Energetics and Reactions*, February 27-March 4, 2005, Ventura, CA.

Charter Member of the Dean's Council for Excellence in the Sciences, College of Arts and Sciences, New Mexico State University, 2004-present

Publications (239 total)

Professor Hase has published extensively in the field of chemical reaction dynamics for the past 35 years. A full list of publications, summaries of current research projects, and animations of chemical and molecular reaction dynamics can be viewed at his group website: http://www.monte.chem.ttu.edu/

Software Development

A General RRKM Program, Quantum Chemistry Program Exchange-234, 1974

Minicomputer Version of QCPE-234, Quantum Chemistry Program Exchange-291, 1975

MERCURY: A General Monte Carlo Classical Trajectory Program, Quantum Chemistry Program Exchange-453, 1983

Academic Computing: A Strategic Plan, Prepared by Wayne State University Academic Computing Policy Committee, 1986

A General RRKM Program, Quantum Chemistry Program Exchange 14, 644 (1994)

VENUS96: A General Chemical Dynamics Computer Program, Quantum Chemistry Program Exchange 16, 671 (1996)

You Can't Get Success if You Don't Get in the Game, Minority Scientists Network: http://www.nextwave.sciencemag.org/miscinet

Graduate Students Obtaining Degrees at Wayne State University

Date	Name	Degree	Field
1977	Thomas, D.W.	M.S.	Chemistry
1977	Wolf, R.J.	M.S.	Chemistry
1980	Wolf, R.J.	Ph.D.	Chemistry
1984	Duchovic, R.J.	Ph.D.	Chemistry
1989	Lu, D.-h.	Ph.D.	Chemistry
1989	Cho, Seon-Woog	Ph.D.	Chemistry
1991	Hu, Xiche	Ph.D.	Chemistry
1993	Zhu, Ling	Ph.D.	Chemistry
1994	Accary, C.	M.S.	Chemistry
1994	Barbarat, P.	M.S.	Chemistry
1995	Peslherbe, Gilles	Ph.D.	Chemistry
1996	de Sainte Claire, Pascal	Ph.D.	Chemistry
1996	Wang, Haobin	Ph.D.	Chemistry
1998	Bosio, Sylvie B.M.	M.S.	Chemistry
2000	Mann, David J.	M.S.	Chemistry
2001	Mann, David J.	Ph.D.	Chemistry
2001	Meroueh, Oussama	Ph.D.	Chemistry
2002	Wang, Yanfei	M.S.	Chemistry
2003	Mehra, Samip	M.S.	Computer Science
2003	Sun, Lipeng	Ph.D.	Chemistry
2003	Yan, Tianying	Ph.D.	Chemistry
2004	Arora, Pratima	M.S.	Computer Science

Postdoctoral Research Fellows and Visitors

Feng, Da-Fei	postdoc	1973–1974
Nagy, Paul	postdoc	1976-1978
Bhalla, K.C.	postdoc	1980–1981
Swamy, K.N.	postdoc	1980–1985
Bhuiyan, Bari	postdoc	1982–1983
Cho, Young June	postdoc	1990–1992
Song, Kihyung	postdoc	1994–1995, 2001
Bolton, Kim	postdoc	1996–1997
Jin, Ryan	postdoc	1997–1999
Sawilowsky, Ellen	postdoc	1998–1999
Li, Guosheng	postdoc	1998–2001
Barker, John R.	visitor	2000
Xie, Hongwei	postdoc	2000–2002
Mazyar, Oleg	postdoc	2003-present
Danailov, Daniel	postdoc	2003–2004
Tasic, Uros	postdoc	2004-present
Vayner, Gregory	postdoc	2004-present
Louderaj, Upakarasamy	postdoc	2004-present
Song, Kihyung	visitor	2004-present
Rahman, Asif	postdoc	2005-present

Hase Collaborators

Prof. Scott L. Anderson, University of Utah

Prof. Tomas Baer, University of North Carolina

Professor John R. Barker, University of Michigan

Prof. V. Chaudhary, Wayne State University

Prof. Ralph Deal, Kalamazoo College

Dr. Charles Doubleday, Jr., Columbia University

Prof. G. Edjalali, Wanye State University

Prof. J.S. Francisco, Purdue University

Prof. M.J. Frisch, Gaussian Inc.

Dr. Jean H. Futrell, Pacific Northwest National Laboratory

Prof. Evelyn M. Goldfield, Wayne State University

Dr. B.C. Garrett, Pacific Northwest National Laboratory

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