THE JOURNAL OF PHYSICAL CHEMISTRY A

 VOLUME 110, NUMBER 4, FEBRUARY 2, 2006

Photo by Kathy B. Jones

Chemical Dynamics Simulations in the Gas Phase and on Complex Surfaces A Tribute to William Hase

It is a great pleasure to introduce this special issue in celebration of Bill Hase's 60th birthday. With this short tribute, it is an honor for us, as friends and former colleagues, to share Bill's scientific accomplishments. The chemical reaction dynamics studied by Bill and his research group cover a wide range of theoretical topics including development and application of the RRKM and variational transition state theories, analytical potential energy surfaces for polyatomic chemical reactions, classical/quasi-classical trajectory simulation techniques, and on-the-fly direct dynamics simulations that interface classical chemical dynamics with electronic structure theories. For many of their simulations, they have used animations to visualize the complex dynamics of multi-atom chemical processes. Bill's research spans many important chemical processes including intramolecular dynamics and unimolecular reactions, bimolecular reactions (e.g., S_N2 reactions), biomolecular reactions, and reactions on complex surfaces and at interfaces. Bill's contributions to the scientific community are broad and multifaceted. In addition to over 200 research publications, Bill has written textbooks, reference books, and many book chapters. In addition, Bill has developed new curricula for generations of students and has inspired and supported many young researchers, including faculty members, to greater success.

Bill's theoretical work began with investigations of RRKM and non-RRKM unimolecular kinetics and the effects of exit-channel coupling on the unimolecular decomposition of a variety of small molecules. As an expert in RRKM theory, a microcanonical transition state theory for unimolecular reactions, Bill published a book chapter entitled "Dynamics of Unimolecular Reactions", in *Modern Theoretical Chemistry*, Vol. 2, ed., W. H. Miller, Plenum Publishing Co., New York, NY (1976), pp 121−170. This chapter has become one of the classic reviews for RRKM theory and for theoretical modeling of unimolecular reactions.

Bill's most renowned work focuses on molecular and chemical reaction dynamics. Over the years, Bill's research

10.1021/jp058282i CCC: $33.50
Published on Web 01/26/2006

group has developed various theoretical methods and practical tools for the computer simulation of chemical reactions. Bill remembers that his first computer program for classical trajectory simulations was written in assembly language and ran on a DEC PDP-10 (an early multi-user mainframe computer). Since that time, Bill's group has been a leader in the development of advanced programs for simulations. Readers of *The Journal of Physical Chemistry* are familiar with performing *ab initio* chemical reaction dynamics on the fly with desktop workstations using VENUS, a general chemical dynamics computer program developed by Bill's group and used by many others in the scientific community. As every computational (and experimental) chemist recognizes, theoretical models are very useful for the proper interpretation of experimental data but are most insightful when they can be used in a predictive fashion. Bill has taken this creed to heart in all of his research endeavors, by applying the computational methods his group has developed to a wide variety of chemical systems. These range from gas-phase unimolecular and bimolecular reactions, to liquids, to collisions of gas-phase ions with surfaces, and structure, adhesion, and friction of interfaces. In the textbook co-authored with Tom Baer, *Unimolecular Reaction Dynamics—Theory and Experiments*, one observes many successful applications of RRKM theory in the interpretation of experimental results.

Another important area of Bill's work deals with dynamics studies of bimolecular reactions. In a series of publications, Bill and his group have elucidated the underlying atomic-level mechanisms that lead to non-statistical behaviors in the kinetics of gas-phase S_N2 reactions. This has provided theoretical interpretations to the seminal experimental work of John Brauman, Michael Bowers, Albert Viggiano, and many others and has stimulated more thorough experimental study of related processes. Further contributions to the understanding of intramolecular dynamics and atomic-level motions associated with S_N2 chemical reactions include non-RRKM behavior as described in *J. Phys. Chem.* **1990**, *94*, 6148, *Science* **1994**, *226*, 998, and *J. Am. Chem. Soc.* **2001**, *123*, 5753.

Despite the complexity of molecular surface interactions, Bill's group has made major contributions to the understanding of energy deposition in collisions of rare gas atoms with hydrocarbon surfaces and fragmentation processes involved in collision-induced and surface-induced dissociation. Using classical trajectory simulations, Bill revealed the detailed dynamics of interaction between molecules and self-assembled monolayers, one of the most in-depth investigations of beam−surface interactions. Our understanding of the structure, energetics, and dynamics of interfaces, including characterization of friction and adhesion at heterogeneous boundaries, has been improved by insightful work from the Hase group. We highlight two papers, *J. Phys. Chem. B* **2002**, *106*, 8029 and *J. Am. Chem. Soc.* **2002**, *124*, 1524, as a window to Bill's work in surface reactions.

As a true academician, Bill's contribution to science is multifaceted. Bill has published over 200 peer-reviewed research papers and 7 review articles. He has also authored 2 books and 23 book chapters. We are certain that every reader, either as a student or as a professor, has used the book Bill co-authored with J. I. Steinfeld and J. S. Francisco entitled *Chemical Kinetics and Dynamics*, currently in its second edition. Bill has had an important influence on many experimental groups through the clarity of his papers and his presentations. We really learned rate theory by reading two of his comprehensive reviews: "Variational Unimolecular Rate Theory", *Acc. Chem. Res.* **1983**, *16*, 258 and "Some Recent Advances and Remaining Questions Regarding Unimolecular Rate Theory", *Acc. Chem. Res.* **1998**, *31*, 659. We can recommend a similar exercise to any researcher who wishes to learn this important theory.

Bill is among the best and most dedicated teachers we have ever known. It is always a great pleasure for us, as his colleagues, to sit in his classroom and observe him inspiring young minds. Over the years, Bill has contributed to 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.

We have come to know Bill very well and quickly became good friends after joining the faculty at Wayne State University as assistant professors of Chemistry in the mid-nineties. Bill sets a great example of a dedicated academician, a true warrior of scientific research regardless of any difficulty or hardship encountered, and an inspiring and loyal friend to researchers all over the world. We invite readers of this Festschrift to glimpse the impact of Bill's gas-phase chemical dynamics work by reading the special issue of the *International Journal of Mass Spectrometry* published in his honor in 2005 (Vol. 241, Nos. 2−3). As a long-term and loyal contributor, reviewer, and editorial advisory board member for the *Journal of Physical Chemistry*, Bill's 60^{th} birthday provides an opportunity to recognize and celebrate a truly deserving physical chemist for his broad impact on theory and computational science as well as experimental chemistry. *Bill's deep understanding of collision theory and chemical dynamics has been put to profitable use in other areas of life and has helped him to become a superb golfer, attaining reproducible single-digit handicap data.* With his new position as the Robert A. Welch Professor of Chemistry at Texas Tech University, one can only imagine where his classical trajectory will lead him in physical chemistry and on the golf course (*will there be any quantum effects?*). May this special issue be the great beginning to this most recent phase of Bill's scientific adventure.

Mary T. Rodgers
Gang-yu Liu

Guest Editors