THE JOURNAL OF PHYSICAL CHEMISTRY A

Special Issue Preface

pubs.acs.org/JPCA

Fifty Years of Chemical Reaction Dynamics

Chemistry is a science of violent transformation. Molecules inhabit a world of enormous electric and magnetic fields where they are torn apart in shattering collisions often yielding huge energy release and unimaginable acceleration. This dynamic upheaval is at the heart of every macroscopic chemical process, from a candle flame to the workings of a neuron. Our ability to understand and predict the behavior of these processes depends entirely on our understanding of the factors controlling these elementary dynamical events. Kinetic studies of chemical reactions, starting at the time of Arrhenius, provide important information on the reaction rates and global trends, but the average over the reactant states obscures key dynamical information: What forces and interactions are driving the reaction? Where do the energy and angular momentum go? Why does this bond break and not that one? Why does this product form and not that one? Although these are questions of profound intellectual interest, this is far more than an academic pursuit. Answers to these questions allow us to extrapolate our knowledge from a domain in which we can comfortably make measurements to the vastly larger space where experiments are not possible. They also enable us to sift through the innumerable reactions taking place in a macroscopic system and identify those that are likely to be most important. Building a thorough understanding of chemical reaction dynamics at the microscopic level requires precise control of both internal and relative energies between reactants during collision as well as detection techniques that allow us to probe the transient products in their newly formed internal states before subsequent collisions have obscured the primary processes. This was made possible with the advent of molecular beam and laser technologies about half a century ago, along with the parallel emergence of powerful theoretical methods and computers. The focus of this field has since been on understanding elementary reactions involving atoms and small molecules in the gas phase at the highest level of detail but is ever expanding into new areas. In this special issue, we celebrate the field of Chemical Reaction Dynamics, rather arbitrarily marking its beginning with the first Conference on the Dynamics of Molecular Collisions (DMC) in 1965.

From the start, a defining feature of the field of chemical reaction dynamics has been the close experimental and theoretical collaboration. Indeed, this is one of a few fields in physical chemistry in which quantum-state resolved attributes are routinely compared between measurements and calculations. The close interplay between experiment and theory has allowed the establishment and testing of new models that deepen our understanding of reaction dynamics and improve our predictive ability. The theory of reactive scattering at the beginning borrowed heavily from nuclear physics but has since developed its own unique characteristics. It is now common for theory to reproduce and sometimes predict accurately experimental observations, particularly for small reactive systems. From its beginnings focused on small-molecule scattering and the comparisons to classical trajectory calculations performed on primitive computers with rudimentary potentials, we now address frontier areas, as seen in the remarkable range of papers in this special issue: nonadiabatic reactions on multiple potential energy surfaces; novel reaction mechanisms that challenge transition-state theories of reactivity; dynamics in liquids and at interfaces; atmospheric and astrochemical reactions; spectroscopic and dynamic probes of catalytic systems and transient reactive intermediates; collisions and reactions in an ultracold world where quantum behavior governs all; and extension of detailed dynamics investigations to large polyatomic molecules. Yet these pursuits are still informed by the principles that shaped the previous investigations: an urgent curiosity, a desire to know where the classical description ends and the quantum one begins, and the urge to be where state-of-the-art experiment meets state-of-the-art theory. The founders of the field have taught us well, and the vibrant state of things is attested to by the 140 or so participants in the most recent DMC meeting as well as the rich and diverse array of papers presented here.

The Conference on the Dynamics of Molecular Collisions has formed a unique platform for researchers in this field and has witnessed its phenomenal growth over the years. The first DMC was held in 1965 in New Hampton, New Hampshire and was chaired by Professor John Fenn, the 2002 Nobel Prize recipient for his work in developing electrospray ionization methods that efficiently introduce biological molecules into molecular beams. The chairman of the second meeting was Professor John Polanyi, the 1986 winner of the Nobel Prize in Chemistry for his work on reaction dynamics. Professor Polanyi shared this Nobel Prize with Professor Dudley Herschbach of Harvard and Professor Y. T. Lee of University of California Berkeley. Professor Lee chaired the seventh DMC meeting in 1978 held at Pacific Grove in California and was the keynote speaker in the 25th DMC held this year. The DMC has also played a key role in educating graduate students and postdoctoral researchers entering this field. It has also served as a gathering place for international cooperation and exchange. We sketch the history of the meeting here:

The History of the Conference on the Dynamics of Molecular Collisions

1965	New Hampton, New Hampshire, John Fenn (Yale University)
1968	Andover, New Hampshire, John C. Polanyi (University of Toronto)
1970	Oak Ridge, Tennessee, E. F. Green (Brown University)
1972	Plymouth, New Hampshire, Sheldon Datz (Oak Ridge National Laboratory)
1974	Santa Cruz, California, James L. Kinsey (Massachusetts Institute of Technology)
1976	Plymouth, New Hampshire, Bruce E. Mahan (University of California)
1978	Pacific Grove, California, Yuan T. Lee (University of California)
1981	Plymouth, New Hampshire, R. James Cross (Yale University)

Special Issue: Dynamics of Molecular Collisions XXV: Fifty Years of Chemical Reaction Dynamics

Published: December 17, 2015

DOI: 10.1021/acs.jpca.5b08530
J. Phys. Chem. A 2015, 119, 11949−11950

1983	Gull Lake, Minnesota, W. Ronald Gentry (University of Minnesota)
1985	Snowbird, Utah, Donald G. Truhlar (University of Minnesota)
1987	Wheeling, West Virginia, Paul Dagdigian (The Johns Hopkins University)
1989	Pacific Grove, California, William H. Miller (University of California)
1991	Lake George, New York, James M. Farrar (University of Rochester)
1993	Helen, Georgia, Joel M. Bowman (Emory University)
1995	Pacific Grove, California, Daniel Neumark (University of California, Berkeley)
1997	Gull Lake, Minnesota, George Schatz (Northwestern University)
1999	Lake Harmony, Pennsylvania, James Valentini (Columbia University)
2001	Copper Mountain, Colorado, James T. Muckerman (Brookhaven National Laboratory)
2003	Granlibakken, California, Laurie J. Butler (University of Chicago)
2005	Pacific Grove, California, Albert Wagner (Argonne National Laboratory)
2007	Santa Fe, New Mexico, David Chandler (Sandia National Laboratory)
2009	Snowbird, Utah, Anne McCoy (The Ohio State University)
2011	Snowbird, Utah, David Nesbitt (JILA/University of Colorado)
2013	Granlibakken, California, Hua Guo (University of New Mexico)
2015	Pacific Grove, California, Arthur Suits (Wayne State University)

Starting in 2007, on the initiative of Dave Chandler at Sandia National Laboratories, the DMC inaugurated the Dudley Herschbach Prize for outstanding contributions to this field by both experimental and theoretical researchers. The design of the medal, shown on the cover of this issue, underscores the close collaboration between experiment and theory. The list of winners of the Herschbach Prize to-date is given below:

2007: Dick Zare and Bill Miller
2009: Dan Neumark and Don Truhlar
2011: Yuan T. Lee and George Schatz
2013: Giacinto Scoles, Peter Toennies, and Joel Bowman
2015: Carl Lineberger and Millard Alexander

It is fitting to mark this anniversary, the 25th DMC meeting, and this milestone, 50 years of reaction dynamics, with a special issue of *The Journal of Physical Chemistry*. We thank Anne McCoy and George Schatz for suggesting this. We would also like to express our gratitude to the past meeting chairs listed above for their inspiring passion and dedication to the field and the students and postdocs for their long labors in these pursuits. The diverse contributions in this special issue provide an up-to-date snapshot of the field. It is clear that experimental research based on the traditional molecular beam continues to reveal novel and surprising dynamics issues, but there are also new frontiers that explore uncharted territory. In the meantime, theoretical developments remain fully engaged with experimental advances to provide the necessary insights into reaction dynamics. We expect many years of future advances in this important field of research in physical chemistry.

Hua Guo
Department of Chemistry, University of New Mexico
Arthur G. Suits
Department of Chemistry, Wayne State University

DOI: 10.1021/acs.jpca.5b08530
J. Phys. Chem. A 2015, 119, 11949−11950