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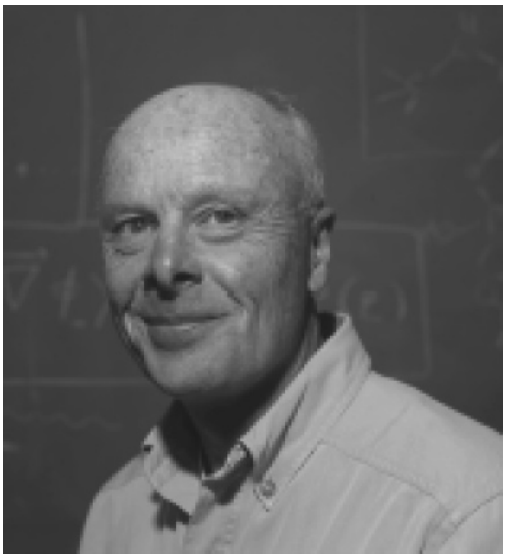

Photo by Margaret Simons

A Tribute to Jack Simons

We are pleased to join the many colleagues who contributed to this special issue of *The Journal of Physical Chemistry A* in dedication to Professor Jack Simons upon the occasion of his 60th birthday. Jack is a theoretical chemist of remarkably broad interests. He has made several important contributions on the algorithmic front, but it is his emphasis on applications of theory to elucidate chemical phenomena where he has made his greatest impact. Jack has a deep understanding and appreciation of experiments, and he has had close collaborations with many experimental researchers (he has over 130 coauthors among his more than 300 publications).

Jack received his undergraduate degree in chemistry in 1967 from Case Institute of Technology. With the support of an NSF Graduate Fellowship, he then joined the group of Professor John Harriman at the University of Wisconsin, Madison, where he did research on reduced density matrices. Jack completed his Ph.D. work in less than three years. He then received an NSF Postdoctoral Fellowship, which he used to pursue work in statistical mechanics under professors John Deutch and Irwin Oppenheim at MIT. After spending one year at MIT, Jack moved to a faculty position in the chemistry department at the University of Utah where he has been ever since. From 1986 to 1989, Jack was Chair of the Department and in 1989 he was made the Henry Eyring Professor of Chemistry.

The start of Jack's academic career coincided with the time when theoretical chemistry was moving from a pencil and paper science to being more computationally oriented. Jack's early work concentrated on negative molecular ions and electron affinities (EA). The calculation of electron affinities by traditional computational quantum chemistry methods is notoriously difficult. Jack was among the pioneers who proposed a radically new approach for directly calculating EAs, avoiding the problems inherent in traditional methods that involve separate calculations on the neutral and anionic molecules. Jack's group not only worked out the formalism of this new approach, they also implemented it in an efficient computer code that they used to study a large number of chemically important species. Today, direct methods similar to Jack's equation of motion (EOM) method are widely used theoretical tools for interpreting experimental photoelectron spectra.

From the mid 70s to early 90s, Jack and his group made major advances in the methodologies of electronic structure calculations with multiconfigurational wave functions. In addition, Jack's contributions have been pivotal in understanding electron−molecule dynamics, where he developed methods for studying

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electron detachment processes that are induced via non-Born−Oppenheimer coupling as well as for characterizing temporary anions and other types of resonances.

Jack has also made important advances to the understanding of chemical bonding. For example, in collaboration with Lai-Sheng Wang of PNNL, and one of us (A.B.), Jack provided the first examples of five-atomic molecules with planar tetracoordinate carbon and has also contributed to the understanding of multiply charged anions.

In addition to Jack's many scientific achievements, he has been an outstanding educator and a caring mentor to several generations of students and postdocs.

Jack has written four popular books: *Second Quantization-Based Methods in Quantum Chemistry* (Academic Press, 1981; with Poul Jorgensen as coauthor); *Energetic Principles of Chemical Reactions* (Jones and Bartlett, 1983); *Quantum Mechanics in Chemistry* (Oxford University Press, 1997, with Jeff Nichols as coauthor); and an *Introduction to Theoretical Chemistry* (Cambridge University Press, 2003).

Jack has pioneered the use of the World Wide Web as a vehicle for communicating the excitement of theoretical chemistry. Jack's web page on theoretical chemistry (http://simons.hec.utah.edu/TheoryPage/index.html) is a valuable source of information for young scientists contemplating a career in theoretical chemistry. In the summer of 2005, Jack ran a very successful workshop on "Computation, Simulation, and Theory in Chemistry, Chemical Biology, and Materials Chemistry" in which he targeted the nonexpert and made the workshop material available via the web (http://simons.hec.utah.edu/school/index.html).

The three of us have been extremely fortunate to have worked with Jack over extended periods of time. One of us (J.N.) started collaborating with Jack as a visiting professor directly after graduate school; another of us (A.B.) spent seven years in Jack's group as a visiting scientist, and the third member of the group of guest editors (K.J.) has known Jack since their days together at MIT. As has been the case with many of Jack's former students, postdocs, and visitors, the three of us have continued to collaborate with Jack on both research and educational ventures. Although the Internet has made it easy for researchers in different parts of the world to carry out productive collaborations, it is not uncommon to find several of Jack's former group members and collaborators frequently returning to Utah for extended stays in Jack's group. Simply put, Jack is a great person with which to discuss science and to try out one's latest ideas. Today's scientists have many demands on their time; writing papers and trying to meet proposal deadlines, juggling committees, reviewing papers and proposals, supervising students and postdocs, and if in an academic setting, teaching. In spending time with Jack and his group, we are reminded that science is fun.

We join with Jack's many other friends and colleagues in wishing him a joyous 60th birthday and many more years of scientific productivity and happiness.

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Kenneth Jordan