Autobiography of Jack Simons

I was born in Youngstown, Ohio, on April 2, 1945, as the first child of Jack W. and Margaret A. Simons. I have three brothers, Tom, Jim, and Bob. My father was an accountant and served in this capacity for the Girard, Ohio, school system. Mom was a mother and homemaker and the kindest human being I have known. Although both of my parents attended college (Mom earned a degree in child psychology), neither was very interested in books, culture, and the like. Grandparents on my father's side came from Wales in the 1880s, with my grandfather working in the coalmines and railroads in West Virginia and Ohio. On my mother's side, my grandparents came from France and Ireland, and my grandfather became a financial executive in the steel industry.

I do not recall why, but I became interested in chemicals and chemistry at an early age. I liked making stuff that exploded or burned with bright colors, and I wondered what characteristics of the chemicals made these things happen. I recall one "experiment" in which I tried to make sulfuric acid by bubbling SO_2 through water. I knew this would make H_2SO_3, but I figured that if I heated the burning liquid sulfur "hard enough", I could form enough SO_3 to generate the desired H_2SO_4. The experiment did not work! My basement caught fire, and my mother cut off my access to my beloved chemistry lab for a full month. Anyway, by the time I was eleven, I knew I wanted to be a chemist; it was a lot of fun and I wanted to understand what it was all about. Fortunately, my father had a friend, Bill Jones, a pharmacist, who could help me acquire chemicals that I could not purchase from Merck or Standard Scientific Supply through the mail. So, I was able to carry out many exciting experiments in the basement of my home through much of my primary- and high-school years.

Very few of the students passing through the Girard school system went to college; most of the boys moved on to jobs in the local steel mills or automobile plants. Moreover, it was not "cool" to display intellectual ability or interest in academic matters, so I had to become a bit of a tough guy and a good pool player to avoid being picked on for doing well in school. I played sports, including baseball (I was a shortstop and brother Tom played third base) and golf (for which I won scholarships to college), which also helped me to fit into the social scene reasonably well.

Even though I was not surrounded by an academic environment, most parents in Girard emphasized going to school, working hard, and doing the right thing. Moreover, I was lucky to encounter some excellent teachers, especially in the high-school years. In particular, Ms. Helen Ebinger (math) and Mr. Herb Cramer (chemistry and physics) treated me wonderfully. They allowed me to come to school early in the morning before classes began when they would tutor me on more advanced material in math and science. Our school had no advanced placement classes, but I think my sessions with these two teachers gave me at least the equivalent. Mr. Cramer also allowed me free reign of the chemistry and physics prep room, so I could carry out whatever experiments I desired. He also shared his experiences in learning about the new Chem Study and PSSC Physics programs that he would offer to students in later years.

When applying to colleges, I knew I wanted to go to a place that was strong in science, but I also knew I had to get a scholarship that paid all tuition, fees, and living expenses because Mom and Dad could not afford to pay. Although golf provided me the opportunity to attend some colleges, they were not of the academic quality I desired. After considering several options and being awarded the needed scholarship, in 1963 I chose to go to Case Institute of Technology in nearby Cleveland and, of course, to major in chemistry. This proved to be a wonderful choice for me because Case provided both the challenges I needed to advance my scholarship and a nurturing environment for this shy and insecure young person. In my first years at Case, I had exceptional educators in chemistry with Malcolm Kenney and John Fackler being two of the best. In my freshman year, I undertook an undergraduate research program with Prof. Gordon Barrow in which we studied the far infrared spectra of tetraalyklammonium tetraphenylboride ion pairs in various solvents. Although these experiments proved interesting and Prof. Barrow found them productive, I soon found myself more interested in trying to invent inter-ion potential functions that would reproduce the observed spectra than in collecting more data. I detected that I liked the theoretical aspects better than the experimental, so in my sophomore year, I decided to pursue research under Prof. Donald Whitman doing electronic structure theory. It was at this stage in my development that I realized I wanted to pursue theoretical chemistry.

After graduating from Case in 1967, I took my NSF Graduate Fellowship and entered the Ph.D. program at the University of Wisconsin, Madison. I chose Wisconsin because there were several faculty members doing theory among whom I could choose an advisor. I eventually chose to work with the youngest theorist, John Harriman, and to work on reduced density matrix theory. John arranged for me to attend the Sanibel Symposium and Winter School as well as a School on many-body theory in Seattle where I met Yngve Öhrn and Jan Linderberg, who later would become special friends. Of course, the director of the Wisconsin theory group, Prof. J. O. Hirschfelder, also mentored me as I progressed through my research program. Joe and his wife, Betty, became good friends to Peg and me and remained so for the remainder of their long lives.

During the first year at Wisconsin, I met a wonderful young woman named Peg Glaspey who was also a chemistry graduate student working with Prof. Claude Woods doing microwave spectroscopy. It turns out Peg's background in quantum mechanics was weak (although she had been both high school and college valedictorian), so I agreed to tutor her in this subject. After a very brief courtship, I asked her to marry me and was extremely fortunate and happy that she said yes. We were married in Madison during the break between the two semesters on January 31, 1968.

The late 60s were a time of great turmoil in America because of the Vietnam war, and Madison was at the center of much of this action. As a young male and eligible for the military draft, I was very nervous about the possibility of having to go to war, so I worked hard to finish all of the Ph.D. requirements quickly. As a result, I was able to graduate in less than three years in 1970 and to earn an NSF Postdoctoral Fellowship, which I used to go to MIT to pursue work in statistical mechanics under Profs. John Deutch (future director of the CIA) and Irwin Oppenheim.

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While at MIT, I met several young scholars who would become some of my primary competition for academic jobs and who have gone on to distinguished scientific careers (Casey Hynes, Dave Freeman, Peter Ortoleva, Tom George, Jimmy Doll, Atilla Szabo, and Niel Ostlund). Although most of my future research lies within the fields of electronic structure and dynamics, building a solid background in statistical mechanics was important to me. This gave me the confidence that I could purse whatever challenges I encountered when using theory to understand chemical phenomena; I could bring to bear methods from whatever areas of theoretical chemistry were needed.

After spending only one year in Cambridge, I was fortunate to be offered a faculty position at the University of Utah. So, at the ripe old age of 26, I chose to join the Utah Chemistry faculty in 1971 because of the presence of Profs. Henry Erying (his Ph.D. student, Joe Hirschfelder, had introduced me to Henry during my time in Madison), Frank Harris (a brilliant leader in electronic structure theory), and Josef Michl (a young hot shot organic chemist who also did excellent theory). Fortunately, I had made the correct choice, and I have been more than pleased to have remained in Utah throughout my career. The excellent Ph.D. students, postdocs, and visitors I had access to as well as the beautiful Utah mountains and canyons, of course, also played a role in this decision, as did the decency with which colleagues at Utah treated me.

Early in my career at Utah, I became interested in negative molecular ions and electron affinities. The experimental study of these species was beginning to undergo a rapid growth and improvement, so I decided this was a direction in which theory could contribute. Having learned about second quantization and many-body theory during my Ph.D. years, I came up with the idea of developing a new approach to compute electron affinities as Bill Miller would say "directly and correctly". It was clear to me that such an approach was important because electron affinities are intensive properties and to compute them by subtracting the total energies (which are extensive properties) of the neutral molecule and of the anion was fraught with danger. With some of my earliest postdocs (Wes Smith and T. T. Chen) and Ph.D. students (Earl Andersen and John Kenney), we developed the equations of motion (EOM) method for computing electron affinities, and we successfully tested this method on several anions. At about this same time, I was fortunate to attract a brilliant postdoc (Poul Jørgensen) who helped us extend the rigor and utility of the EOM method and who has collaborated with me at several stages over our careers, including writing a textbook on second quantization methods. At about the same time another exceptional scientist, Ken Jordan, whom I had met at MIT, came to work with me prior to beginning his own academic career at Yale, and he got me interested in studying electrons binding to highly polar molecules. This evolved into a long-time study of so-called dipole-bound anions, and, much to my benefit, collaborations with Ken continue to this day. These efforts blossomed largely through the efforts of two postdocs who also became long-time collaborators, Maciej Gutowski and Piotr Skurski, and their scientific progeny.

Between the mid 70s and early 90s, our group pursued several fruitful avenues of research of a methodological nature including development of new approaches for the study of multiconfigurational and other multi-reference wave functions (Esper Dalgaard, Jørgensen, Ajit Banerjee, Debashis Mukherjee, Jim Jensen, Ron Shepard, Bill Fink, and Mark Hoffmann), walking "uphill" to find reaction transition states using eigenvector following methods (Jeff Nichols, Jørgensen, Hugh Taylor, Judy Ozment, and Peter Schmidt), and calculating analytical gradients and Hessians for correlated wave functions (Jørgensen, Jerry Boatz, Keld Bak, Trygve Helgaker, and Martin Feyereisen).

Our studies of molecular anions studied experimentally by our friends, John Brauman and Carl Lineberger, led us to develop new methods for studying how vibration−rotation to electronic energy flow induces electron detachment via non-Born−Oppenheimer coupling (Grzegorz Chalasinski, Prabhat Acharya, Rick Kendall, and Doug O'Neal). Because many of the anions we studied are metastable with respect to electron loss, we also had to learn how to treat such states within the framework of conventional electronic structure theory. This led us to exploit stabilization and complex coordinate rotation methods to compute energies and lifetimes (Zlatko Bacic, Bob Donnelly, Egon Nielsen, David Chuljian, Gina Frey, Joel Liebman, Danny Yeager, and Per Kaijser) of metastable electronic and vibration-rotation states. Later, we even extended these studies to resonances and cross-sections of ion−molecule reactions (Rich Bell and Mike Salazar).

In more recent years, our interests evolved away from methodological issues toward applications to especially interesting chemical problems. Again I was very lucky when a distinguished scientist, Alex Boldyrev, came to work with me, because he played a major role in this evolution. He expanded our horizons into the study of small molecular clusters, and multiply charged ions that have unusual bonding character (Ed Earl, Ramon Hernandez, Nick Gonzales, and Vince Ortiz), and this remained a significant component of our efforts for some time. With Alex, we also studied how Rydberg orbitals can be used to form bonds, and with Maciej Gutowski, we studied how two electrons can enter molecular Rydberg orbitals to form so-called double-Rydberg anions.

More recently, we have become involved with studying how low-energy electrons cause damage to DNA and how they cause positively charged peptides to fragment by cleaving very specific bonds (Iwona Anusiewicz, Piotr Skurski and his Ph.D. students, Agnieszka Sawicka, Monika Sobczyk, and Joanna Berdys) in gas-phase mass spectroscopy experiments.

I think that because my interest has always been more toward chemistry than in theory (e.g., I describe myself as a theoretical chemist, but stress that chemist is the noun and theoretical is the adjective), more of the group's work has involved studying molecular phenomena and unusual species than developing new theoretical tools. We have not been shy to apply existing methods but have come up with new ideas when needed, always relying on a good background in electronic structure, dynamics, and statistical mechanics. As a result, in addition to the fields of major emphasis discussed above, we have undertaken research projects that do not fall under one of these umbrellas, and some very fine students, postdocs, and visitors have contributed to these studies (Jeanne Mchale, Mark Roberson, Veronika Nefedova, Wim Cardoen, Sam Datta, George Purvis, Jeppe Olsen, Jim Anchell, Xiao Wang, Monique Chacon, Anthony Ketvirtis, Jens Oddershede, Berta Fernandez, and Jacek Jakowski). There have also been a significant number of experimental and theoretical colleagues with whom my research group has been fortunate to collaborate on a variety of topics; for all of these opportunities I am very grateful.

In addition to these research activities, involvements in educational outreach efforts have given me special joy. The textbooks I wrote with Jeff Nichols and Poul Jørgensen stand out, as does my involvement in organizing many conferences and schools and in writing and maintaining the web site on theoretical chemistry (http://simons.hec.utah.edu/TheoryPage).

As I look back at all of the happy times I have had doing science with so many talented people, I understand how blessed I have been, and I look forward to a lot more scientific excitement in the years to come. Thanks much to all the nice people who have contributed to this collection of scientific papers; I am proud to have had a chance to work with all of you.

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