

Autobiography of William A. Lester, Jr.

Born and raised on the south side of Chicago, I was the second child and only son of the four children of William A. and Elizabeth Lester. My father was a mailman for many years before becoming a postal supervisor. During the early years, my mother was at home and was often to be found making clothes for my sisters, Florence, the oldest, and Judith and Karen. Later she sewed professionally before becoming a physician's assistant.

My grandparents were an important influence in my life. My maternal grandfather was college educated having earned a bachelor's degree at Atlanta University. He attended a different law school (Ohio State University, Northwestern University, and the University of Wisconsin, Madison) for each of 3 years of study because of the need to take time off to work between terms. He passed the Illinois Bar, and during my childhood was awarded a plaque for 50 years of the practice of law in Cook County (Chicago). A kind man with a droll sense of humor, he emphasized to me, in many ways, the importance of getting things done. My maternal grandmother was also college educated having attended Morris Brown College in Atlanta, Georgia. My maternal grandmother was a practical nurse who prepared for the profession by attending night school in Chicago. My paternal grandfather died before I was born. Both sets of grandparents came to Chicago from the Atlanta, Georgia, area—my mother's family before 1910 and father's family during the great migration of Black people to the North in 1917.

All of my elementary school education was in public schools with totally Black student populations owing to the racial segregation in housing that dominated the city at that time. Shortly after World War II, my family moved to a new housing development on the far south side of the city. The new neighborhood elementary school fed its students into a previously all white high school. As a consequence, Florence and I were among the earliest Black students to attend Calumet High School.

I was a good student in elementary and high school. I skipped two grades in elementary school and attended summer school 1 year that led to my entering high school at age 12. I was on the honor roll in elementary school, a member of the junior and national honor societies in high school and a participant in a variety of extracurricular activities in the latter. My favorite course in high school was chemistry, a subject I had investigated as a sophomore for an English course assignment to describe one's future vocation.

Along with my academic interests, I also liked sports, especially basketball and football. Because of my size and speed, or rather lack thereof, I was unable to make the football team but I did have some success in basketball. Although I barely made the high school basketball team my junior year, practice over the intervening summer coupled with a growth spurt of 3 in., and development of a jump shot, led to my becoming a starting guard on the varsity team as a senior.

A major turning point occurred for me during my senior year of high school when, at the suggestion of friends, I sought part-time employment at the University of Chicago. Armed with typing skills gained my junior year, I was successful in being hired by the UC Department of Physics as a technical typist for ONR (Office of Naval Research) research reports. The head

of the laboratory, The Laboratory for Molecular Structure and Spectra (LMSS), was Robert Mulliken and second in command was Clemens Roothaan. I held various responsibilities in that office during my undergraduate and master's degree studies.

Although I had decided in high school to pursue chemistry as my college major I also enjoyed history and did well in the subject in high school. The latter point is worth mentioning because I applied for admission and financial aid to several widely recognized universities in the Chicago area, but without success. I did have the good fortune, however, of gaining admission and a scholarship to the University of Chicago through a unique arrangement at my high school. A former librarian, Victoria A. Adams, had established a scholarship to the University of Chicago that required satisfactory performance on a history examination. It was the V. A. Adams Scholarship that provided my passage to the University of Chicago.

Although I was a serious chemistry student during my undergraduate years, basketball presented a competing interest. The University of Chicago's basketball team had only won one game and lost 47 over the 3-year period immediately prior to the arrival of my class in 1953. With three fellow freshmen and a returning senior in the starting lineup, we were able to turn around the fortunes of UC basketball and win half our games that first year. In my succeeding 3 years of eligibility, we posted similar records. During my UC basketball career, I started every game after the first one of my freshman season. I was selected captain for 3 years and broke the single game scoring record twice. Two records are still standing: season average (25.5) and most field goals in a game (19).

My achievements as an undergraduate led to a number of awards. These included the Amos Alonzo Stagg Medal given to the outstanding scholar-athlete, and the "Man of the Year" award, both in 1957.

The value of a graduate degree was clear to me from the exposure made possible by my Physics Department position. Upon completion of my undergraduate studies in 1958, however, I was unable to gain admission to the premier graduate programs in chemistry in the country. After consultation with the Chemistry Department Chair, Henry Taube, he stated that the best master's degree I could earn would be one from Chicago and permitted me to stay on to study for the degree, which was atypical for the period, i.e., to stay for an advanced degree at the same institution that you received your bachelor's degree, and to pursue a master's degree. I completed requirements for the master's with a research project carried out under the direction of Stuart Rice. With the award of a teaching assistantship to Washington University in St. Louis, I began doctoral studies at that institution in the fall of 1959.

The academic year 1959–60 held not only a move to St. Louis, but marriage to Rochelle Reed during the Christmas break. Upon learning during the spring semester that I would not be able to pursue a doctorate with the person of my choice, I applied to The Catholic University of America (CUA) in Washington, D.C., to continue my doctoral studies. The CUA had also awarded me a teaching assistantship the previous year, but I did not receive the award letter until after the deadline for acceptance. Rochelle and I remained in St. Louis through the summer before departing for Washington, D.C. My plan at CUA was to study under Virginia Griffing, an arrangement suggested

by Bernard Ransil, a Research Associate with Mulliken who had earned his doctorate from CUA under Griffing's direction. I had gotten to know Bernie well by assisting him in data preparation at LMSS for the computational studies that he published in the well-known 1960 issue of *Rev. Mod. Phys.*, that served as the proceedings of the 1959 Boulder Conference on Theoretical Chemistry.

Graduate study progressed well at CUA, but the modest teaching assistant salary led me to seek outside employment during the summer of 1961 to counter the living costs of an impending family of four in Washington, D.C. Rochelle had given birth to William III in early 1961, I learned from Ransil that graduate student summer appointments were possible at the National Bureau of Standards (NBS), now National Institute of Standards and Technology. He suggested that I contact Morris Krauss who he knew from NBS. The result of this contact was my appointment to NBS as a summer intern in 1961. I returned to CUA for the academic year 1961–1962 to complete campus course and exam requirements, and to pursue a dissertation problem. The untimely death of Griffing during the Spring of 1962 and Krauss's interest in my returning to NBS culminated in my appointment to the NBS staff as a physical chemist, a position I held through the completion of doctoral requirements.

The years at NBS provided me with an exceptional learning experience. I shared an office with Krauss and a new postdoctoral associate, Frederick Mies, recently arrived from Brown University. These interactions and those with other NBS scientists provided a stimulating intellectual environment and enabled me to gain an appreciation of research not commonly obtained as a graduate student.

I completed my doctoral dissertation in November 1964 on the calculation of molecular properties using Boys's recently published correlated Gaussian functions. I was then successful in obtaining a postdoctoral appointment with Richard Bernstein at the Theoretical Chemistry Institute, University of Wisconsin, Madison, and took an educational leave of absence from NBS. Dick introduced me to the strongly coupled rotational excitation problem that was a fertile area and my springboard into collision theory.

After only 8 months as a Research Associate in the Theoretical Chemistry Institute, I was asked to assume the position of Assistant Director of the Institute owing to Dan Konawalow's departure to a faculty position. The position would involve handling administrative matters of the Institute including responsibility for processing postdoctoral applications. I accepted the position, which offered the prospect of learning about the inner workings of an internationally recognized research organization even though it significantly reduced time for research. A year later I was also appointed Lecturer in the Department of Chemistry, University of Wisconsin, which was my first collegiate teaching position, and resigned my NBS position.

In 1968 I joined the professional staff of the IBM Research Laboratory in San Jose, California, to pursue research in quantum chemistry and molecular collisions. I was hired into the recently created Large Scale Scientific Computations Department under the leadership of Enrico Clementi. In the Department were a number of researchers whom I knew from my University of Chicago student days. These included Doug McLean, who had been a graduate student when I was first hired at LMSS, and the late Megumu Yoshimine. Paul Bagus, who I first met when we were in the same general physics course as undergraduates, also joined the Department during that first month. Robert Nesbet was already a veteran of the Laboratory

when I arrived. Around the same time Douglas Henderson and the late John Barker joined the Department. It was an exciting time not only because of the brilliant lab co-workers but also because I now had sufficient computational resources to calculate converged scattering cross sections. I had been only able to compute selected partial waves because of the limited computer access in Madison. Furthermore, the Research Laboratory's computer resources enabled me to compute potential energy surfaces for collisional energy transfer using *ab initio* methods, which contrasted sharply with the practice at the time of constructing potential energy surfaces using semiempirical methods.

This early IBM period was one in which Clementi created the IBM World Trade Postdoctoral Program that brought research associates from Western European countries to the San Jose Laboratory. I had the pleasure to work under this program with John Mulder, Joachim Schaefer, Frank Rebenrost, and Reinhard Schinke. In addition, owing to the kind consideration of UC Berkeley chemistry faculty members William Miller and Henry Schaefer III, two Berkeley graduate students, Barbara Garrison and Andy Raczskowski, worked with me at the San Jose Research Laboratory. The late Sheldon Greene was also a frequent visitor working with the late Bowen Liu as well as myself on a number of projects. Research with Garrison, Greene, and Miller led to resolving the origin of anomalous cooling of H_2CO in the interstellar medium. There were many laboratory colleagues with whom strong friendships developed for which space does not permit me to list.

In 1975 I moved to the IBM T. J. Watson Research Center in Yorktown Heights, New York, to serve on the Technical Planning Staff, a support function to Ralph Gomory, IBM Vice President and Director of Research, IBM Research Division. My area of responsibility on the staff was science for the three IBM Research Division laboratories—Yorktown Heights, San Jose, and Zurich. In 1976 I returned to the San Jose Laboratory as manager of the molecular interactions group.

In 1978, after a national search, I was selected as Director, National Resource for Computation in Chemistry (NRCC), housed at the University of California's Lawrence Berkeley Laboratory (LBL). In that position I organized and directed the first national research effort in chemistry, concentrating on improving computational efforts of chemists by making available information on new computational methods, developing computational algorithms and related software, and conducting research in chemistry that utilized computational methods. I also held concurrently the position of Associate Director of LBL.

In 1981 I was appointed Professor, Department of Chemistry, University of California, Berkeley. Prior to joining the faculty, I was introduced to the quantum Monte Carlo method by the person I had hired to be responsible for statistical mechanics for the NRCC. I am referring here to David Ceperley who, while holding an NRCC appointment, worked with Bernie Alder on the application of QMC to the electron gas. This work produced the original exchange correlation functional that was to give density functional theory a major boost. Ceperley and Alder's success with recovery of 100% of the correlation energy of the system led me to propose a project of computation of selected molecules to serve as a test of the approach for chemical systems. Peter Reynolds joined the NRCC staff in the final year of the organization to enable completion of this project. The high quality of the computed energies from this study led me change my research focus fully to QMC.

At the request of Neal Lane, with whom I had a common research interest on the coupled-channel approach to rotational excitation in the sixties, I moved to the National Science Foundation in early 1995 under the IPA (Intergovernmental Personnel Act). Neal had become NSF Director and sought my involvement to assist his administration in the area of human resources. I was appointed Senior Fellow for Science and Engineering and Assistant to the Director for Human Resource Development. I held this position until December 1996 when I returned to UC Berkeley. Neal moved on to the White House as the President Clinton's Science Advisor.

The early and succeeding years on the Berkeley faculty led to research interactions with a number of brilliant students and postdoctoral and research associates who are listed separately. I cannot overstate the wonderful interactions and productive research that were an outgrowth of these contacts.

During all of these professional activities, I have had the unwavering support of my wife Rochelle. We raised two wonderful children, William III and Allison, and we have been blessed with four delightful grandsons: William IV (Alex) and Austin, and Charles (Tré) and Chandler.

William A. Lester, Jr.