Theor Chim Acta (1992) 82: 3–6

Theoretica Chimica Acta

Joseph O. Hirschfelder[1]

Joseph O. Hirschfelder belongs to the founders of modern theoretical chemistry. Over five and one-half decades, his research has covered a wide range of scientific areas: chemical kinetics, chemical applications of quantum mechanics, structure of liquids, intermolecular forces, combustion, nuclear explosions, kinetic theory of gases, quantum mechanical perturbation theory, and laser chemistry.

'Joe' – as he was known to everyone – was born on May 27, 1911, in Baltimore, Maryland. He did his undergraduate work at the Universities of Minnesota and

[1] Adapted from *Biographical Memoirs*, National Academy of Science (to be published). This account was prepared by three of his former students and colleagues, Professors R. Byron Bird, Phillip R. Certain, and Charles F. Curtiss, all of the University of Wisconsin-Madison

Yale and he received two Ph.D.s from Princeton in 1936, working in theoretical chemistry with Henry Eyring and in theoretical physics with Eugene Wigner. He spent an additional year at Princeton as a postdoctoral fellow with John von Neumann at the Institute for Advanced Studies, while also continuing his cooperation with Eyring and H. S. Taylor. During this time, he worked on surprisingly many fundamental problems, including the polarizability of the hydrogen molecule and the hydrogen molecule ion, suggested by E. U. Condon; the separation of the rotational coordinates from the N-particle Schrödinger equation with E. P. Wigner; the energy of the H_3 molecule and the H_3^+ molecule ion with Eyring and N. Rosen; the a priori calculation of the reaction rate between molecular and atomic hydrogen with Eyring; a free-volume theory of liquids with Eyring, and applications of the viral theorem to the scaling of wave functions.

In 1937, he went to the University of Wisconsin as a research associate, where he became an instructor in physics in 1940 and an assistant professor in chemistry in 1941. He continued his research on intermolecular forces and chemical kinetics, and began a program to relate intermolecular forces to the properties of gases.

During World War II, he developed a system of interior ballistics for guns and rockets, and, as a group leader in the Los Alamos atomic bomb project, was the first to predict fallout from atomic explosions. He was the chief phenomenologist at the Bikini bomb test in 1946 and, after the war, chaired the editorial board that produced the 1950 book *The Effects of Atomic Weapons*. These experiences exposed him to a myriad of practical problems and led him to become a theoretician with a strong interest in experimental facts and phenomena who imparted to his graduate students a genuine concern for being able to interpret theoretical results in a form useful to experimentalists.

Upon returning to Wisconsin in 1946, he established the University of Wisconsin Naval Research Laboratory, whose agenda included experimental as well as theoretical studies, one of the main activities being the study of flames and explosions. It had great impact on subsequent flame structure studies and led to one of the earliest publications dealing with what is now called singular perturbation theory.

By 1950, Hirschfelder decided to summarize this work and integrate it with information from other sources. The result was *The Molecular Theory of Gases and Liquids*, written in collaboration with his colleagues and former students Charles F. Curtiss and R. Byron Bird and published in 1954. Its widespread influence was reflected by *Current Contents* listing it as the fourth most cited scientific reference for the period 1961–1972. While writing it, Hirschfelder came to the conclusion that further progress in the prediction of the properties of gases and liquids depended on knowledge about intermolecular forces obtainable only from a priori calculations. He became a pioneer in this field even before its later expansion through the use of computers. He investigated the use of hypervirial theorems, developed ideas on the use of perturbation and variational theories to obtain upper and lower bounds, and extended perturbation theory to almost degenerate states.

In the early 1960s, as part of the Apollo effort to reach the moon, the National Aeronautics and Space Administration invited Professor Hirschfelder to present

a proposal to convert the Naval Research Laboratory into the Theoretical Chemistry Institute in order to investigate intermolecular forces and chemical dynamics. This led to an expansion of staff and facilities, including the creation of an experimental program in molecular beam scattering under R. B. Bernstein. The interdisciplinary emphasis with theory tied closely to experiment was characteristic of Joe's approach to science. It was also during this period that he collaborated closely with Per-Olov Löwdin of Uppsala and the University of Florida.

From 1963 to 1968, the Theoretical Chemistry Institute grew rapidly, with a large number of graduate students, postdoctoral fellows, and visiting faculty coming to Madison. Joe's and Betty's keen interest in people and generous hospitality (Joe had married the mathematician Elizabeth Stafford Sokolnikoff in 1953) created an atmosphere of lively scientific exchange and cooperation among the leading theoretical and experimental chemists of the world. The three principal areas of theoretical research were the theory of intermolecular forces, particularly the development of exchange perturbation theory including the Pauli principle; the theory of elastic, inelastic, and reactive molecular scattering; and the statistical mechanics of real gases.

During the 1970s, Hirschfelder began a longtime association with the University of California at Santa Barbara. His research interests turned to the interaction of light with matter, and the nonlinear effects associated with intense lasers. After his retirement in 1981, he continued to interact with colleagues and pursue research, splitting his time between Madison and Santa Barbara.

A good example of the vitality of Joe's intellect was his response to receiving radiation treatments for a tumor on his spine. Intrigued by how the radiation could destroy the tumor without damaging the spinal cord, he asked the medical physicists about the mathematics used to focus the radiation. The equations reminded him of those used in weather satellite tracking and, consequently, he put the medical physicists in touch with a former postdoctoral associate, Robert Pyzalski, then working in meterology. Not only was Pyzalski able to be helpful to the medical physicists but, in fact, meterology lost him to medical physics, where he could devote his research efforts to helping people.

Joseph O. Hirschfelder directed the Ph.D. research of 39 students, and collaborated with over 100 postdoctoral fellows and visiting professors. His students and their students have received Ph.D.s in more than 15 different fields of science and engineering.[2] His feelings about breadth in the scientific enterprise are best reflected in his own words[3]:

> "... In industrial and government laboratories, interdisciplinary problems are solved by task forces of people having different skills and backgrounds. Frankly, I am very much concerned that the training we give our students is so highly specialized that they are not prepared to

---

[2] C. F. Curtiss, R. B. Bird, P. R. Certain (1982) *J. Phys. Chem.* 86:6A–8A; on p. 8A there is an academic genealogy showing Joe's academic children, grandchildren, etc

[3] J. O. Hirschfelder, "The Scientific and Technological Miracle at Los Alamos", pp. 67–88 of Reminiscences of Los Alamos 1943–45. L. Badash, J. O. Hirschfelder, H. P. Broida (eds.) Dordrecht, The Netherlands: D. Reidel Publishing Company, 1980

> tackle problems that are not closely connected with their theses. It is important that our students develop sufficient breadth that they can explain their ideas to people with different backgrounds. This is essential if they are to become useful members of an interdisciplinary task force."

Professor Hirschfelder received the Debye Award of the American Chemical Society (1966), the Edgerton Gold Medal of the Combustion Institute (1966), the Silver Medal of the American Society of Mechanical Engineers (1981), and the National Medal of Science from President Ford (1976). He was elected to the National Academy of Sciences (1953), the American Academy of Arts and Sciences (1959), the Norwegian Royal Society (1965), and the Royal Society of Chemistry of Great Britain (1981). He received honorary degrees from Marquette University (1978) and the University of Southern California (1980).

Joe died peacefully in his sleep at his home on March 30, 1990, after a valiant 2-year struggle with cancer. His creation, the Theoretical Chemistry Institute, continues to flourish. Its director, James L. Skinner, now carries the title Joseph O. Hirschfelder Professor of Theoretical Chemistry.

Phillip R. Certain[1]