# John Anthony Pople

The most fundamental change in the chemical sciences in the second half of the 20th century might well have been the growth of computational chemistry into a major way of understanding molecular behavior. This significant conceptual and practical advance was enabled by the work of many pioneers, but John Anthony Pople's ideas and contributions powered the development of computational science in chemistry. His greatest achievement (other than his close-knit family) was the development of tools that changed the way chemists and other scientists interested in molecules do chemistry. He died in Chicago of liver cancer on 15 March 2004.

Born in Burnham-on-Sea, England, on 31 October 1925, John studied at Cambridge University. There, he received his bachelor's degree in 1946 and PhD in 1951.

Following postdoctoral fellowship work at Cambridge, he joined the National Physical Laboratory in Teddington, England, as its scientific director. He immigrated to the US in 1964—his move was memorialized by a London evening newspaper with the headline "Another Brain down the Drain"—where he became the J. C. Warner University Professor of Science at the Carnegie Institute of Technology (now Carnegie Mellon University). He left Carnegie Mellon to take a position as Trustees Professor of Chemistry at Northwestern University, where he remained until his death.

John's chief and abiding interests were in molecules—what they do and why they do it. His early interests were in mathematics. After grammar school, he never took a formal chemistry course. Indeed, when he first applied for membership in the American Chemical Society, he was rejected because he lacked chemical experience. That lack clearly was not a stumbling block in his career, given that he, with Walter Kohn, was awarded the Nobel Prize in Chemistry in 1998. His PhD thesis work with John Lennard-Jones was devoted to developing theoretical models, including electronic structure models, to explain some of the remarkable and unique experimental properties of water. The thesis contained insightful and creative partial explanations of the many unique properties of water. That experimental basis for theoretical challenge was a hallmark of John's work throughout his career.


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The areas of science in which John worked were numerous. His accomplishments included elucidating the competition between vibronic coupling and spin–orbit coupling; the first study of vibrational modes in molecular crystals; the first suggested systematic approach to determining localized molecular orbitals; comparisons of valence-bond to molecular-orbital theory; the modeling of polymer structures and relaxations; proposing charge defect motion (now often called soliton motion) in molecular solids; and developing some of the first models in semiempirical molecular orbital theory. His book *High-Resolution Nuclear Magnetic Resonance* (McGraw-Hill, 1959), written with coauthors W. G. Schneider and H. J. Bernstein, was the first bible of that field.

John was a combination of visionary and builder, mathematician and computer scientist, chemist and entrepreneur, teacher and inspirer. He took his inspirations and ideas where he found them; the idea for ring currents to explain chemical shifts in aromatic hydrocarbons came from a conversation with Bernstein as they waited for an airplane. John often initially attacked a topic by thinking about experimental problems and defining the simplest model to explain a given behavior. From that simplest picture, he gradually, artfully, and insightfully built a more sophisticated and accurate scheme.

His greatest contributions lie in the insights he provided, in the students he trained, and in the methods he developed and shaped. The most striking methods lie in ab initio electronic structure theory. John took as his challenge the development of techniques and tools to allow scientists and engineers to understand molecular electronic structure. Such development required major advances, including overcoming the electron correlation problem, providing reliable basis sets for actual calculations, norming computation methodologies against reliable experimental data, and constructing and making available a set of robust and efficient software codes. John accomplished all of those.

Notations devised by John and colleagues, such as MP2 theory in the 6-31G* basis set, are familiar to molecular scientists worldwide. The MP2 describes the type and level of perturbative corrections to the self-consistent field method, and the 6-31G* describes the one-electron basis set. John and his group took delivery of the third VAX minicomputer ever made, and thus began a trend away from central processors toward workstations. The group also produced Gaussian 68, the first widely applicable code for molecular electronic structure calculations. He and his students wrote, optimized, and commercialized many software tools that changed the way scientists do chemistry.

John's science was marked by great rigor and economy; he kept it simple, sharp, and brilliant. He was a humble man of astounding insight and clarity of thought who had incredible range and depth, and remarkable warmth. One image that comes to mind as an example of his humility was when he got down on the floor and crawled to play with a colleague's two-year-old child. A direct man, he was also incisive and had a subtle sense of humor and clipped and articulate speech. He was a supportive and treasured colleague. One of the last projects on which he was engaged, an improved definition of the second law of thermodynamics, began when he challenged a colleague to calculate the entropy of a fried egg.

John won many awards. He was made a Knight Commander of the Most Excellent Order of the British Empire in 2003 and was a fellow of the Royal Society and many other academies.

John is missed tremendously by the community of molecular scientists, his colleagues, former students and postdocs, and 4 children and 11 grandchildren. His contributions continue whenever a biochemist in Bangalore, or a geologist in Sydney, or a chemical engineer in Glasgow uses one of John's software packages to help understand the behavior of a molecule and thereby the behavior of the physical world.

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## Philip Hauge Abelson

Few have been so fortunate as Philip Hauge Abelson to simultaneously possess a brilliant mind, a passion for science and its role in human affairs, and a commitment to celebrating scientific progress while goading scientists on to higher aspirations. Born on 27 April 1913 in Tacoma, Washington, he lived life to its fullest, right up to the time he succumbed to pneumonia in Washington, DC, on 1 August 2004. Phil is missed and will be remembered as one of the giants of the 20th-century physics community.

Phil received his BS in chemistry (1933) and MS in physics (1935) at Washington State College (now University). He decided to pursue additional graduate work at the Radiation Laboratory at the University of California, Berkeley, where he received his PhD in nuclear physics in 1939. He subsequently joined the Carnegie Institution of Washington (CIW) as an assistant physicist. In 1940, he embarked on a short vacation, during which he visited the Radiation Lab. He and Edwin McMillan's mutual research interests became apparent and they decided to work together. While exploring nuclear fission, the pair discovered neptunium.

Phil left CIW to join the Naval Research Laboratory in 1941. Swept up in the Manhattan Project, he drew on the chemistry background he had obtained during his undergraduate days at Washington State and developed a process to produce gaseous uranium hexafluoride ($UF_6$), a key step in isotopic separation of uranium isotopes. He also prepared the first feasibility study of nuclear-powered submarines.

After World War II, Phil rejoined CIW, where he directed the Geophysical Laboratory (1953–71) and became the institute's president (1971–78). During his time at Carnegie, he discovered amino acids in fossils more than 100 million years old.

A researcher of many talents and extraordinary energy, Phil gave most generously of his time. He added to his work at CIW: He became the editor of *Science* (1962–84) and was a central figure in the evolution of the American Association for the Advancement of Science. His thought-provoking editorials demonstrated both his prodigious capacity to stay abreast of diverse developments in science and technology and his keen insights about the increasing imperative to link the S&T community more effectively to public policymakers and to society in general.

Phil frequently used the editorial pages of *Science* to report to the S&T community, policymakers, and citizens the results and implications of studies—especially those carried out by the Congressional Office of Technology Assessment. Those editorials provide a still-fresh panorama of the status and prospects of global conditions deeply connected to human aspirations, and the need and opportunities for S&T to contribute in a positive way.

I'm reminded of the following saying: "When all is said and done, more has been said than done." Phil knew that one answer to that lamentation is to repeatedly lay the matters before the people until action is taken. He also was an inveterate optimist. One of his notable publications was a collection of essays entitled "Enough of Pessimism!" As the director of the Con-