

## Obituary

## John A. Pople (1925–2004)

Sir John Pople died on 15 March 2004 at the age of 78. He was a giant in his chosen field, computational quantum chemistry, for which he was awarded the Nobel Prize in Chemistry in 1998. Pople revolutionized the way chemistry is practised today by making it possible to carry out research in the computer as a complement to the conventional chemistry of the laboratory. It was Pople who was most responsible for making computational quantum chemistry available to the community of chemists at large, and he dominated the scene in this area during the past five decades.

Pople was born in Burnham-on-Sea in south-west England in 1925. His talents in mathematics were apparent at an early age. However, he describes in his Nobel autobiography how he introduced deliberate errors into his mathematics exercises at Bristol Grammar School so as not to appear too clever. It was not until a new mathematics teacher arrived, and set a particularly challenging test, that he succumbed to temptation and turned in a perfect paper, including multiple solutions to several of the problems. Despite the remarkable achievements that were to follow, he never lost his modest manner.

Pople went on to study mathematics and physics at the University of Cambridge. But eventually his interest in pure mathematics began to wane and he decided to apply his mathematical skills to chemistry. The germs of the ideas that were to provide the focus for his life's work — developing mathematical models that could describe all of chemistry — were sown in 1952. There were some digressions, including early seminal contributions and a classic text in the then-emerging field of nuclear magnetic resonance, work that was a forerunner to the magnetic resonance imaging of today. But the main game was always the creation of models for studying chemistry.

It was known long ago, and enunciated by Paul Dirac in 1929, that the laws of quantum mechanics could in principle be used to predict all of chemistry. What Pople did was convert this to a practical reality. His aim was to enable chemists to straightforwardly predict the properties of molecules, such as molecular structures and the way molecules react with one another, by using a computer rather than by carrying out experiments.

He went about this task by first formulating the essential characteristics of an acceptable theoretical model. For



### Innovator in computational chemistry

example, it should be unique, well defined, unbiased, objective and widely applicable, as well as satisfying certain, more technical, requirements (such as being 'size-consistent'). If the model performed satisfactorily in systematic comparisons with experimental data, it could then be used to make predictions in cases where experimental data are not available.

Pople then proceeded to design a series of theoretical procedures that could serve as the basis for the model. In some cases, he was the inventor or co-inventor of the new procedures — for example, the Pariser–Parr–Pople  $\pi$ -electron theory of the 1950s, or 'complete neglect of differential overlap' (CNDO) and other 'semi-empirical' theories of the 1960s. In others, he reformulated existing ideas, such as Møller–Plesset perturbation theory, to make them practically and objectively applicable to a wide cross-section of chemistry.

A key to implementing such procedures was the construction of efficient computer programs, and this was one of Pople's major contributions. His development and release of the Gaussian 70 program marked a turning point in the field, making it possible to carry out broad theoretical studies on real chemical problems on a scale that had not previously been possible. This was also the hallmark of Pople's subsequent computational initiatives. Even in the more recently popularized density functional theory, where he was formally

only a minor player (the dominant contributor being Walter Kohn, with whom Pople shared the Nobel prize), he systematized the way such calculations were carried out and incorporated them into the Gaussian program. This undoubtedly helped significantly in accelerating the widespread acceptance and use of density functional theory in chemistry.

Computational quantum chemistry is used today by myriad chemists across a variety of fields. It has become a viable adjunct to experiment, and is used in solving fundamental problems. It is also being increasingly applied by industrial companies in more practical situations, such as the design of new drugs and new materials. It is especially valuable in studying substances that might be difficult to examine experimentally, for instance because they have a very short lifetime or are toxic or explosive. The computer is oblivious to such hazards.

The success of computational chemistry has of course been helped by massive and continuing increases in computer power. The computer available to Pople in 1970, when Gaussian 70 was born, was a CDC 1604. A standard personal computer today is roughly 100,000 times faster, has 5,000 times as much memory, and yet costs several hundred times less.

Apart from being a brilliant researcher, Pople was also a great communicator, as anyone who heard him lecture will know. Some people have the knack of making simple things complicated. Pople kept simple things simple, and had the gift of making complicated material appear simple as well.

Virtually all of Pople's prizewinning work was carried out while he was a professor at Carnegie–Mellon University in Pittsburgh, Pennsylvania, from 1964 to 1993, although it continued after he moved to Northwestern University in Evanston, Illinois. He also had close connections with the Australian National University in Canberra, which he described as his second academic home, and which he visited on nine occasions during the 1980s and 1990s. His death is a great loss not only for science but also for his many friends and colleagues.

John Pople was married to Joy Bowers in 1952. They shared a close relationship for just under 50 years before Joy passed away in 2002. He is survived by his four children, 11 grandchildren and one great-granddaughter.

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