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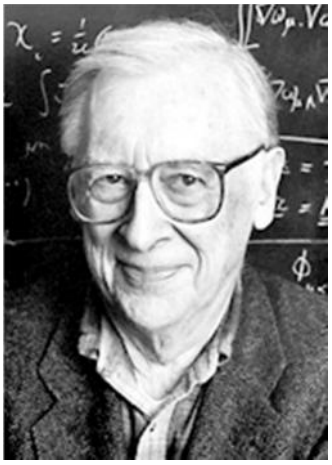
Nobel Prize in Chemistry 1998

Walter Kohn



John A. Pople

The Nobel Prize in Chemistry 1998 was divided equally between Walter Kohn *"for his development of the density-functional theory"* and John A. Pople *"for his development of computational methods in quantum chemistry"*.

Information about winners:

Walter Kohn,

University of California at Santa Barbara, USA and,

John A. Pople,

Northwestern University, Evanston, Illinois, USA (British citizen).

RESEARCH INFORMATION:

Development of computational methods in chemistry awarded

Researchers have long sought methods for understanding how bonds between the atoms in molecules function. With such methods it would be possible to calculate the properties of molecules and the interplay between them. The growth of quantum mechanics in physics at the beginning of the 1900s opened new possibilities, but applications within chemistry were long in coming. It was not practically possible to handle

the complicated mathematical relations of quantum mechanics for such complex systems as molecules.

One of the founders of quantum physics, Dirac, expressed the problem in 1929 as follows: "The fundamental laws necessary for the mathematical treatment of large parts of physics and the whole of chemistry are thus fully known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved.

Things began to move at the beginning of the 1960s when computers came into use for solving these equations and quantum chemistry (the application of quantum mechanics to chemical problems) emerged as a new branch of chemistry. As we approach the end of the 1990s we are seeing the result of an enormous theoretical and computational development, and the consequences are revolutionising the whole of chemistry. **Walter Kohn** and **John Pople** are the two most prominent figures in this process. W.Kohn's theoretical work has formed the basis for simplifying the mathematics in descriptions of the bonding of atoms, a prerequisite for many of today's calculations. J. Pople developed the entire quantum-chemical methodology now used in various branches of chemistry.

Computer-based calculations are now used generally to supplement experimental technics. For several decades they have been developed and refined so that it is now possible to analyse the structure and properties of matter in detail. Conventional calculation of the properties of molecules is based on a description of the motion of individual electrons. For this reason, such methods are mathematically very complicated. **Walter Kohn** showed that it is not necessary to consider the motion of each individual electron: it suffices to know the average number of electrons located at any one point in space. This has led to a computationally simpler method, the *density-functional theory*. The simplicity of the method makes it possible to study very large molecules. Today, for example, calculations can be used to explain how enzymatic reactions occur. It has taken more than thirty years for a large number of researchers to render these calculations practicable, and the method is now one of the most widely used in quantum chemistry.

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John Pople is rewarded for developing computational methods making possible the theoretical study of molecules, their properties and how they act together in chemical reactions. These methods are based on the fundamental laws of quantum mechanics as defined by, among others, the physicist E. Schrödinger. A computer is fed with particulars of a molecule or a chemical reaction and the output is a description of the properties of that molecule or how a chemical reaction may take place. The result is often used to illustrate or explain the results of different kinds of experiment. Pople made his computational technics easily accessible to researchers by designing the GAUSSIAN computer program. The first version was published in 1970. The program has since been developed and is now used by thousands of chemists in universities and commercial companies the world over.

Quantum chemistry - a background

The laws of quantum mechanics as formulated more than 70 years ago make it theoretically possible to understand and calculate how electrons and atomic nuclei interact to build up matter in all its forms. The task of quantum chemistry is to exploit this knowledge to describe the molecular system. This has proved easier said than done. It was not until the beginning of the 1960s that development really started, when two events became decisive. One was the development of an entirely new theory for describing the spatial distribution of electrons, and the other was the use of the increasing potential offered by the computer. **Walter Kohn** showed in 1964 that the total energy for a system described by the laws of quantum mechanics can be theoretically calculated if the electrons' spatial distribution (*electron density*) is known. The question is only how the energy depends on the density. Kohn gave important clues based on what this dependence looked like in an imaginary system with free electrons. It was to take several decades and contributions from many researchers, however, before the equation for determining the energy was sufficiently accurately mapped to permit large-scale studies of molecular systems. This has taken place partly through the adaptation of a small number of variables to experimental data. The method Kohn introduced came to be known as the *density-functional theory*. It is now used in studies of numerous chemical problem areas, from

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calculating the geometrical structure of molecules (i.e. bonding distance and angles) to mapping chemical reactions.

During the 1960s many research groups in Europe and the USA started feverishly to exploit the great potential of the computer. New methods of computation were developed and refined. **John Pople** was a leading figure in this field. He realised that if theoretical methods were to gain any significance within chemistry it was necessary to know how accurate the results are in any given case. In addition, they must be easy to use and not too demanding of resources. Through significant improvements in the theoretical methodology at the end of the 1960s Pople designed a computer program which at a number of decisive points was superior to others' efforts. The prerequisites mentioned above could now be fulfilled and GAUSSIAN-70, as the program was called, very soon became widely used. Pople continued during the 1970s and 1980s to refine the methodology, at the same time building up a well-documented *model chemistry*. Here he was able at the beginning of the 1990s to include Kohn's density-functional theory. By these means new possibilities opened up for analysing ever-more complex molecules.

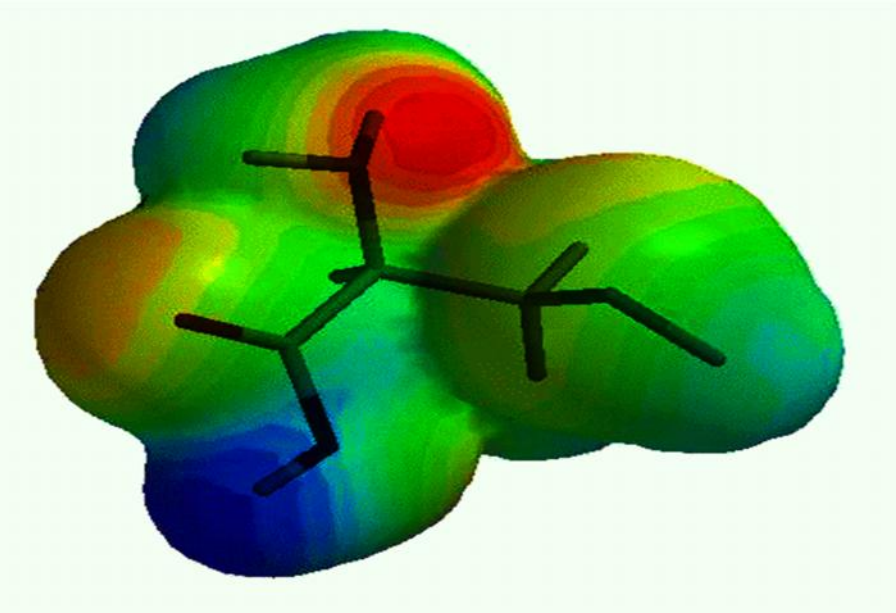

Fig. 1. Electron density in the amino acid cystein calculated using a quantum-chemistry computer program. The picture shows the surface where the electron density is

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0.002 electrons/Å^3 (meaning that nearly all electrons are inside the surface). The grey scale shows the electrostatic potential at this surface, darker portions representing negative potential.

Applications of quantum chemistry

Quantum chemistry is today used within all branches of chemistry and molecular physics. As well as producing quantitative information on molecules and their interactions, the theory also affords deeper understanding of molecular processes that cannot be obtained from experiments alone. Theory and experimentation combine today in the search for understanding of the inner structure of matter. How is then a quantum-chemical calculation carried out?

Let us take the example of the amino acid cystein, illustrated above. How do we produce that image? We sit in front of the computer and start the quantum chemistry program. From the menu we select a molecule in which a carbon atom (C) is bound to a hydrogen atom (H), an amino group (NH_2), a thiolathomethyl group CH_2SH) and a carboxyl group (COOH). The computer draws a rough picture of the molecule on the screen. We now instruct the computer to determine the geometry of the molecule with a quantum-chemical calculation. This can take a minute or so if we are content with a rough result, but up to a day if we desire high accuracy. The screen picture gradually changes towards greater accuracy up to a predetermined level. When this operation is finished we can ask the computer to calculate different properties for the system. In the illustration above we have calculated a surface with constant electron density. The surface is coloured according to the value of the electrostatic potential. This can be used, for example, to predict how the molecule interacts with other molecules and charges in its environment. Such information may be used to study how proteins (which are built up of amino acids) interact with different substrates, e.g. in pharmaceuticals.

Another example may be taken from the universe, in which, apart from stars and planets, there are great quantities of interstellar matter, often collected in vast clouds. What does this matter consist of? It can be studied from the Earth through the radiation the

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molecules emit. The radiation occurs because the molecules rotate. Hence it is possible using the frequency spectrum of the radiation to determine the composition and appearance of the molecules. This, however, is an immensely difficult task, particularly since these molecules cannot always be produced in the laboratory so as to obtain material for comparative studies. Quantum chemistry, however, does not suffer from such limitations. Calculations based on assumed structures can give information on radio emission frequencies that can be directly compared with data collected by the radio telescope. In this way, theory and measurement together can give information on the molecular composition of interstellar matter.

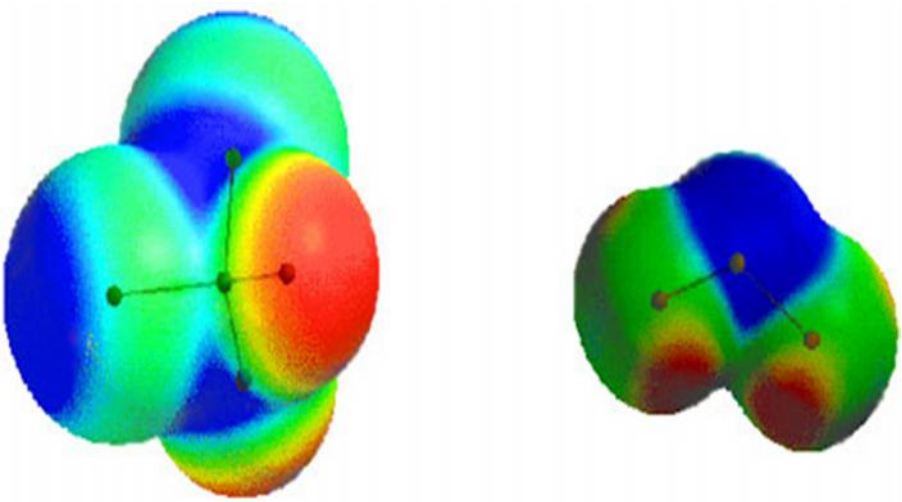

Fig 2. High up in the atmosphere, CF_2Cl_2 molecules (freon, left in picture) are destroyed by ultraviolet light. Free chlorine atoms are formed, which react with O_3 molecules (ozone, right in picture) and destroy them. The process can be studied using quantum-chemical calculations.

Another example. High up in the atmosphere there is a thin layer of ozone molecules that protect us from ultra-violet radiation from the sun. Substances that we release into the atmosphere (e.g. freons) can lead to the destruction of the ozone layer. How does it happen? Which chemical reactions are involved? With quantum-chemical computation we can describe them in detail and thus understand them. This knowledge may help us to take steps to make our atmosphere cleaner.

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Quantum chemistry is used nowadays in practically all branches of chemistry, always with the aim of increasing our knowledge of the inner structure of matter. The scientific work of Walter Kohn and John Pople has been crucial for the development of this new field of research.

For more details please visit:

http://www.nobelprize.org/nobel_prizes/chemistry/laureates/1998/press.html