Fukui's Frontiers

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The first Japanese scientist to win a Nobel Prize introduced the concept of frontier orbitals.

In high school, chemistry was not one of Kenichi Fukui's favorite subjects. He loved mathematics, and was also considered a literary scholar, known for his great love of books and languages. But in 1981, Fukui became the first Japanese scientist to receive the Nobel Prize in Chemistry, for his frontier orbital theory of chemical reactivity. Based on his research on the specific properties of electronic orbitals, Fukui's theory transformed scientists' ability to predict the routes and products of chemical reactions.

Born in Nara, Japan, in 1918, Fukui was the eldest of three sons born to Ryokichi and Chie Fukui. His father, Ryokichi, was a foreign trade merchant and factory manager. Although he was not enamored of chemistry, Fukui took the advice of a respected professor and entered the Department of Industrial Chemistry at Kyoto University, thus beginning a lifelong affiliation with the school. After obtaining a B.A. in engineering in 1941, he accepted a position with the Japanese Army Fuel Laboratory, where he participated in Japan's World War II effort by developing synthetic fuels. He returned to Kyoto University in 1943 and became a lecturer in the Fuel Chemistry Department.

Simultaneously, he began work on his doctoral degree. Rising through the academic ranks, he became an assistant professor in 1945, received his Ph.D. in chemical engineering in 1948, and achieved the rank of full professor in 1951.

Although Fukui was trained as an engineer and had done applied fuel research, he developed an interest in quantum chemistry. He became a largely self-taught theoretician and actively pursued this interest soon after returning to Kyoto University. By 1956, Fukui had gathered around him a group of experimentalists and theoreticians who went on to produce more than 450 papers over the next 30 years, among which were some that dealt with the electronic theory of organic reactions. Other papers were about the statistical theory of gelation, organic synthesis by inorganic salts, and polymerization kinetics and catalysts. Fukui also continued to work in experimental organic chemistry and published 137 papers on the subject between 1944 and 1972.

Kenichi Fukui at a 1981 Nobel Prize committee reception.

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"Delightful Discovery"

In 1952, Fukui published the first paper detailing his theoretical work on the relationship between molecular orbitals (MO) and chemical reactivity. He had found a correlation between the frontier electron density and the chemical reactivity in aromatic hydrocarbons (he referred to this as a "delightful discovery"). This paper provided a simplified theoretical basis for American Nobel Laureate Robert Mulliken's findings on charge transfer and electron donor acceptors in complex chemical structures. Fukui believed that a reaction should occur at the position of largest electron density in the frontier (highest occupied or lowest unoccupied) orbitals. Because many experimental chemists at that time did not have the necessary mathematical background to understand its potential, and because many theoretical chemists thought the idea too simplistic, the paper was largely ignored.

Undeterred, Fukui and his colleagues continued to broaden their theories and experiments and published two more important papers in 1954. In the first of these papers, Fukui included nucleophilic and free-radical attack on conjugated hydrocarbons in his methods. He showed that these could be correlated respectively with the substrate position having the greatest virtual electron density—the lowest unoccupied molecular orbital (which was later called LUMO).

In the mid-1960s, Fukui and Roald Hoffmann (a Polish-born American chemist) discovered—almost simultaneously and independently of each other—that symmetry properties of frontier orbitals could explain certain reaction courses that had previously been difficult to understand. This gave rise to unusually intensive research activity—both theoretical and practical—in many parts of the world.

Fukui developed the theory that during chemical reactions molecules share loosely bonded electrons, which occupy so-called frontier orbitals. This theory advanced the understanding of the mechanism of chemical reactions, especially in the production of organic compounds. Fukui showed that certain properties of the orbits of the most loosely bound electrons and of the "most easily accessible" unoccupied electronic orbitals (which he called "frontier orbitals") had unexpected significance for the chemical reactivity of molecules.

Building on his frontier orbital research, Fukui expanded his research into formulating the path of chemical reactions, and he published his first paper on the topic in 1970. In his autobiography listed on the Nobel website (*www.nobel.se/chemistry/laureates/1981/fukui-autobio.html*), he commented on the findings in this paper: "This simple idea served to provide information on the geometrical shape of reacting molecules, and I was able to make the role of the frontier orbitals in chemical reactions more distinct through visualization, by drawing their diagrams."

Fukui shared the 1981 Nobel Prize in Chemistry with Roald Hoffmann for their theories on the course of chemical reactions. Known for his calm demeanor, Fukui was said to be gracious but composed when informed that he won this prestigious prize. "I am just another chemist scholar," he said, and feared that the publicity would disrupt his commitment to a peaceful existence.

Although his earliest paper outlining the theories of frontier orbitals was ignored, Fukui's (and Hoffmann's) method of attacking difficult and complicated problems succeeded because they made generalizations through simplifications. Today, their method of conceiving the course of chemical reactions is used by, among others, chemists studying life processes and chemists making new drugs. Pharmaceutical and fine chemical companies use Fukui's ideas and methods to predict optimum conditions for a particular reaction pathway and to minimize unwanted side reactions. This level of analysis enables pharmaceutical and chemical manufacturers to yield highly specific and pure products.

Honors Accrue

By the end of the 1960s, Fukui had earned an international reputation as a respected scientist. In 1970, he taught at the Illinois Institute of Technology as a National Science Foundation senior foreign scientist. In 1981, the year he won the Nobel Prize, he was named a foreign fellow of the National Academy of Science. The following year, Fukui was named both professor emeritus of Kyoto University and president of the Kyoto Institute of Technology. He served as president of the Chemical Society of Japan from March 1983 to February 1984. In addition, Fukui was known for his efforts to promote science education in Japan during the later years of his life and was the director of the Institute for Fundamental Chemistry (Kyoto) from 1988 to 1998.

Fukui died of cancer at the age of 79 in January 1998. His obituary in *The Independent,* a London newspaper, remembers Fukui as a "modest, retiring man who hated any kind of publicity. He led a quiet life with his family and a few friends, with whom he loved to drink sake and to play music, for he was an excellent singer of French and German songs."

"I must confess that, when I was writing the 1952 paper, I never imagined I would be coming to Stockholm to receive the Nobel Prize 30 years later," he wrote in his autobiography. "The possibility became a reality through the good circumstances in which I found myself: with my teachers, my colleagues and students, and of course, my parents and family."

Further Reading

Fukui, K., Fujimoto, H., Eds. *Frontier Orbitals and Reaction Paths: Selected Papers of Kenichi Fukui;* World Scientific Publishing Co.: Singapore, 1997.

Autobiographical sketch for the Nobel e-Museum; www.nobel.se/chemistry/laureates/1981/fukui-autobio.html.

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