# From Fuel Chemistry to Quantum Chemistry: Kenichi Fukui and the Rise of the Kyoto School[1]

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Kenichi Fukui (1918–1998) was the first Japanese Nobel laureate in chemistry. He received the 1981 Nobel Prize for his frontier orbital theory, which clarified the mechanism and course of chemical reactions in terms of quantum mechanics. Roald Hoffmann who developed the principle of the conservation of orbital symmetry or the so-called "Woodward-Hoffmann rule" shared the award. Their joint award was the third Nobel Prize in the field of quantum chemistry, following the award received by Linus Pauling (1954) and Robert Mulliken (1966).

The frontier orbital theory is considered by many chemists to be one of the most important conceptual advances in the 1950s in the field of chemical sciences.[2] Despite its historical significance, the literature on the history of quantum chemistry has long been silent about Fukui and his work. Kostas Gavrogru and Anna Simões' recent book, *Neither Physics Nor Chemistry: A History of Quantum Chemistry* (2012), deals with the history of quantum chemistry from the 1920s to the 1970s, but contains no mention of Fukui at all.[3] Today, I would like to talk about Fukui and his quantum chemistry from one perspective, namely, the rise of pure science in an applied academic setting.

When Fukui was awarded the Nobel Prize, there was some confusion about his professional identity among Western media and the people in the scientific realm. *Chemical and Engineering News* erroneously described him as a physics professor of Kyoto University.[4] In addition, the secretary of the Royal Swedish Academy asked whether Fukui was a student of Hideki Yukawa (1907–1981), Japan's first Nobel laureate in physics.[5] Yukawa was a physics professor in Kyoto University, but Fukui was not his disciple.

The confusion seems to have sprung due to the gap between affiliation and accomplishment. Throughout his long career, Fukui belonged to the Faculty of Engineering in Kyoto University, and not the Faculty of Science, which had both the chemistry department and the physics department. He was a professor in the Department of Fuel Chemistry. With this background, why was Fukui able to pursue pure science like quantum chemistry in such a strongly applied academic setting? How could he have established a world-renowned research school of theoretical chemistry there?

James Barthoromew has provided one answer to these questions.[6] In his paper,

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1 Some aspects of this paper have been discussed in Yasu Furukawa, "Nenryo-kagaku kara ryoshi-kagaku e: Fukui Kenichi to Kyoto gakuha no mohitotu no tenkai (From Fuel Chemistry to Quantum Chemistry: Kenichi Fukui and a New Development of the Kyoto School)," *Kagakushi*, vol.41 (2014): 181–233.

2 *E.g.*, Scott A. Davis, "Kenichi Fukui, 1981," in Frank N. Magill, ed., *The Nobel Prize Winners*, vol.3: *Chemistry* (Pasadena, CA: Salem Press, 1990), pp. 1061–1067, on p.1063.

3 Kostas Gavrogru and Ana Simões, *Neither Physics nor Chemistry: A History of Quantum Chemistry* (Cambridge, Massachusetts: The MIT Press, 2012). E. Thomas Strom and Angela K. Wilson, eds., *Pioneers of Quantum Chemistry* (Washington, D.C.: American Chemical Society, 2013) mentions Fukui's name only once.

4 "Five Win Nobels for Chemistry, Physics," *Chemical and Engineering News*, vol.59, no.43 (1981): 6–7, on p. 6.

5 *Fukui Kenichi hakase kinenn gyouji kiroku-shu* (Record of the Dr. Keniichi Fukui Memorial Ceremony) (Kyoto University, 1998), p.7.

6 James Bartholomew, "Perspectives on Science and Technology in Japan: The Career of Fukui Ken'ichi," *Historia Scientiarum*, Vol.4 (1994): 47–54.

"Perspectives on Science and Technology in Japan: The Career of Fukui Ken'ichi," he relates the case of Fukui to Japan's unique historical experience with modern science and technology. In the West, the tendency to stress the distinctions between science and technology has been very strong. By contrast, from the Meiji Restoration period in 1868 onward, the Japanese have adopted Western science and technology as one unified field of research, without considering the difference between the two cognitive domains.

This way of thinking has affected Japan's institutional systems. For example, the University of Tokyo, founded in 1877, taught several engineering specialties, together with physics, mathematics, and chemistry in a single unit prior to the establishment of separate faculties in 1885. Fukui's institution, Kyoto University, was founded in 1897. It, too, made do with a single Faculty of Science and Engineering during its formative years. In 1913, the original faculty was made into two separate faculties: the Faculty of Science and the Faculty of Engineering. In Japan's universities, the Engineering Faculty often received more funds than the Science Faculty. As Bartholomew states, "Fukui was materially better off in the Faculty of Engineering than he might have been in the Faculty of Science."[7] Given this background, it is not surprising that a pure scientist like Fukui emerged from Japan's Engineering Faculty.

However, if this thesis stands good, the same could also be said about the engineering faculties in Japan's other universities (including Tokyo, Tohoku, Kyushu, Hokkaido, Osaka, and Nagoya). In reality, the case of Fukui is exceptional. The University of Tokyo, for example, produced a few talented quantum chemists before World War II. They were either from the Department of Physics (*e.g.*, Masao Kotani) or the Department of Chemistry (*e.g.*, San-ichiro Mizushima) in the Faculty of Science. Chemists of Tokyo's large Department of Applied Chemistry in the Faculty of Engineering were probably materially better off than those of the Department of Chemistry in the Faculty of Science. However, no quantum chemists had come from the Department of Applied Chemistry.

To answer the above questions, then, it is essential to look into Fukui's own talent and career as well as the peculiar environment in which he pursued quantum chemistry.

**The Making of a Domestic Quantum Chemist**

Unlike earlier generations of Japanese scientists, Fukui had no opportunities to study abroad, as his student days and early career in chemistry concurred with the wartime. He later labeled himself as a purely domestic scholar.[8]

Fukui was born in 1918 in Nara, a province nearby Kyoto. As a high school student, Fukui's interest turned to mathematics and physics. He favored mathematics, because of its logical rigor and simplicity. By contrast, he disliked chemistry as it appeared to him as too empirical, nonmathematical, and far from theoretical. He thought of enrolling in the Faculty of Science at Kyoto Imperial University (renamed Kyoto University in 1947) and to major in physics. However, when it was time for him to enter the university in 1938, he applied and was accepted to the Department of Industrial Chemistry in Kyoto's Engineering Faculty instead. This department dealt with very practical subjects, like fibers, rubber, coal, petroleum, and plastics. His decision was based on advice he had received from Gen-itsu

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[7] *Ibid*., p. 52.

[8] Kenichi Fukui, "Wastashi no rirekisho (My Curriculum Vitae)," *Watashi no rirekisho: kagaku no kyudosha* (My Curriculum Vitae: Seekers of Science)(Tokyo: Nikkei shinbun-sha, 2007), 119―226, on p.171. On Fukui, see also Kenichi Fukui, *Gakumon no sozo* (Creation of Scholarship), (Tokyo: Kosei shuppan-sha, 1984);Tokio Yamabe, ed., *Kagaku to watashi* (Chemistry and I) (Kyoto: Kagaku dojin, 1982); Teijiro Yonezawa and Chikayoshi Nagata, eds., *Noberu-sho no shuhen: Fukui Kenichi hakase to Kyoto daigaku no jiyu na gakufu* (The Surroundings of Nobel Prize: Dr. Kenichi Fukui and the Liberal Academic Style of Kyoto University), (Kyoto: Kagaku-dojin, 1999); and James B. Bartholomew, "Fukui, Ken'ichi," *New Dictionary of Scientific Biography*, ed. by Noretta Koertge, vol. 3 (Detroit: Thomson Gale, 2007), pp. 85–89.

Kita (1883–1952), a distant relative and lifelong mentor who impressed him greatly. Fukui sensed Kita's insight that chemistry would become based more and more on physics and mathematics. His insight about the future of chemistry proved correct.

Kita had built up a tradition that stressed the importance of basic research in applied chemistry in the Faculty of Engineering at Kyoto Imperial University.[9] He graduated from the Department of Applied Chemistry in Tokyo Imperial University in 1906. Right after his graduation, he served there as an associate professor for nine years. However, due to a conflict with his boss and his discontent with the department's practically-oriented teaching program, he left Tokyo for Kyoto in 1916. He maintained a sense of rivalry against Tokyo Imperial University. At Kyoto Imperial University's newly created Department of Industrial Chemistry, Kita realized his educational ideal, which stressed pure chemistry as the basis for applied chemistry.

During Fukui's undergraduate days, students of industrial chemistry were required to take courses in basic chemistry such as organic chemistry, inorganic chemistry, and physical chemistry in the Department of Chemistry of the Faculty of Science. The applied chemistry building was located next to the pure chemistry building. This geographical setting helped promote exchange between the two departments. This setting was in contrast with the setting at Tokyo Imperial University where the department of pure chemistry and the department of applied chemistry were separated both geographically and institutionally.

Aware of Fukui's distinct talent for mathematics, Kita further encouraged the undergraduate to learn fundamental science beyond chemistry. Fukui chose to study physics and to focus on quantum mechanics as a newly emerging fundamental science during that time. At that period, quantum mechanics was not taught even in the physics department. Fukui enjoyed teaching himself the subject by reading Erwin Schrödinger's famous papers in *Annalen der Physik*[10] as well as books such *as Handbuch der Physik* from the library of the Physics Department. He also read *Einführung in die Quantenchemie*, one of the earliest textbooks on quantum chemistry written by the exiled German scientist, Hans Hellmann[11]. Now, Fukui was convinced that quantum mechanics was a powerful means of mathematizing and theorizing chemistry. He also believed that it could be used in diminishing the empirical traits of chemistry. Fukui later recalled that the liberal atmosphere in Kyoto had a profound influence on his ideas.[12]

Fukui worked on his senior thesis under the guidance of Haruo Shingu (1913–1988), a young associate professor. The experimental study assigned to Fukui was the synthesis of isooctane which was used for raising the octane number of aircraft fuel. This experience aroused his interest in the chemical reaction of paraffinic hydrocarbons.

During this time, Fukui encountered Shingu's Japanese translation of Erick Hückel's famous lecture on the significance of the new quantum theory for chemistry.[13] The translation was published in a faculty bulletin. Hückle had delivered that lecture at the National Meeting of German Chemists which was held in Münich in 1936. In this lecture,

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9 Yasu Furukawa, "Kita Genitsu to Kyoto gakuha no keisei (Genitsu Kita and Kyoto School's Formation)," *Kagakushi*, vol.35 (2010): 1–17.

10 E. Schrödinger, "Quantiesierung als Eigenwertproblem (Erste Mitteilung)," *Annalen der Physik*, ser.4, 79 (1926): 361–376; *idem*., "Quantiesierung als Eigenwertproblem (Zweite Mitteilung)," *ibid*., 4, 79 (1926): 489–527; *idem*., "Quantiesierung als Eigenwertproblem (Dritte Mitteilung: Störungstheorie, mit Anwendung auf den Starkeffekt der Balmerlinien)," *ibid*., 4, 80 (1926): 437–490; *idem*., "Quantiesierung als Eigenwertproblem (Vierte Mitteilung)," *ibid*., 4, 81 (1926): 109–139.

11 Hans Hellmann, *Einführing in die Quantenchemie* (Leipzig und Wien: Deuticke, 1937).

12 "Science and Technology in Japan," *New Scientist*, 21 March 1985, 30–35, on p. 31.

13 E. Hückel, "Shin ryoshi rikigaku no kagaku ni taisusru imi," trans. By Haruo Shingu, *Kagaku Hyoron*, Vol.3, No.3 (1938) : 115–121 ; Erich Hückel, "Die Bedeutung der neuen Quantentheorie für die Chemie," *Zeitschrift für die Chemie*, Bd.42, Nr.9 (1936): 657–662.

Hückel stated that there was a big gap between theoretical physicists and organic chemists. He said that the former should know more about actual chemistry, while the latter should learn more about new quantum mechanics. He also said that each group should apply then their specialized knowledge in their field. In all likelihood, Fukui was encouraged by this lecture. He wished to bridge the gap between theoretical physicists and organic chemists as an applied chemist.

In 1939, during Fukui's sophomore year, the Department of Fuel Chemistry was created as an expansion of the Department of Industrial Chemistry. At this time, Kita, who became its first chair, directed a large national project of synthetic fuel based on the Fischer-Tropsch method. As a graduate student, Fukui studied under Shinjiro Kodama (1906–1996), another loyal protégé of Kita, in the Department of Fuel Chemistry. Kodama had studied at the Kaiser Wilhelm Institute for Physical Chemistry and Electrochemistry in Berlin in the early 1930s. There, he was influenced by Michel Polanyi who asked him to learn the quantum theory to be able to conduct chemical research.[14] Back in Kyoto, Kodama proposed that Kita hire a physicist who would teach mathematics and quantum mechanics to applied chemistry students. Consequently, the theoretical physicist Gentaro Araki (1902-1980) was employed as a fulltime professor in the applied chemistry section of the Engineering Faculty, an appointment that surprised Japan's chemical community. Kita and Kodama thus created a unique environment that would encourage Fukui's research in quantum chemistry.

## The Frontier Orbital Theory

Thanks to Kita and Kodama's arrangements, Fukui was exempted from the military draft during the war. Instead, he was allocated to engage in the Army Fuel Laboratory in Tokyo. There, he joined wartime research on the synthesis of gasoline additives from butanol (made by the fermentation of sugar), which aroused his deep interest in the reaction of olefinic hydrocarbon compounds. Aside from laboratory work, he was fortunate to spare ample time reading English and German books on quantum physics in the laboratory's well-equipped library.

In 1945, shortly before the end of the war, Fukui became an associate professor of fuel chemistry in Kyoto. One characteristic of the Japanese national university system was the *koza* system. *Koza* is a teaching and research unit consisting of a fixed hierarchy of one full professor, one associate professor, and one or two assistants. The inflexibility of the system sometimes caused problems, but the professor there at the time encouraged Fukui to work on his own research. As Fukui recalled, "Being allowed to be independent and pursue my own work at an early age was a major reason I could become what I am."[15] In 1951, while he was in his early thirties, he was promoted to full professor. Now, he has gained more administrative power.

While teaching applied subjects such as fuel engineering and industrial physical chemistry, he focused his investigative efforts on his long-cherished study: the quantum-mechanical understanding of the chemical reactions of hydrocarbon compounds. His interest in reactions was in contrast to Mizushima's group of theoretical chemistry at Tokyo University where the molecular structure was the main focus of research.[16]

Shingu helped Fukui to recognize the limits of the then dominant electronic theory of organic reactions, the theory developed by the English chemists Robert Robinson and Christopher Ingold. Fukui chose familiar aromatic hydrocarbons as the first object of his

[14] Shinjiro Kodama, *Kenkyu kaihatsu eno michi* (The Path to Research and Development) (Tokyo: Tokyo kagaku dojin, 1978).

[15] "Science and Technology in Japan" (note 12), p.31.

[16] Mizushima's students at Tokyo's Department of Chemistry included Yonezo Morino and Saburo Nagakura.

investigation. The reactivity of naphthalene, for example, could not be sufficiently explained by the Robinson-Ingold electronic theory. The electrophilic substitution in the naphthalene molecule （like the nitration） predominantly yields α-substituted-derivatives. The reason behind this phenomenon was not clear.

Like other quantum chemists, Fukui considered the electron to be the critical entity in chemical reactions. He adopted the molecular orbital approach developed by Hückle and others. However, he “tried to attack this problem in a way that was at that time slightly unusual.”[17] Fukui assumed that the molecular orbital with the highest energy level should play a crucial role in chemical reactions. Using the molecular orbital method, he manually calculated the electron density of the naphthalene molecule and found that the density was largest at the position of α where a chemical reaction took place. With the help of his graduate student Teijiro Yonezawa (1923-2008), he proceeded to calculate by using a mecahnical calculator the density of more complex hydrocarbons such as anthracene, pyrene, and perylene one by one. They found that his initial assumption perfectly coincided with empirical data. He recalled that to his surprise, no one else had ever conceived of such a simple mechanism.[18]

In 1952 Fukui began publishing a series of papers on the frontier orbital theory of reactions in the *Journal of Chemical Physics*.[19] There, he went on to propose that the highest occupied molecular orbital (HOMO) of one reactant and the lowest unoccupied molecular orbital (LUMO) of the other play a dominant role in chemical reactions. These two particular orbitals were referred to as frontier orbitals. He argued that the progress of a reaction depends on the geometries and relative energies of the HOMO and the LUMO frontier orbitals. During the 1950s and early 1960s, Fukui and his coworkers continued to refine and extend his theory.

Initially, the frontier orbital theory was either ignored or attacked. Its highly mathematical expressions were beyond the comprehension of many organic chemists of the time. To those who had been working in the forefront of quantum chemistry, Fukui was totally a stranger. His theory received critical comments from theoretical chemists, such as Harry Greenwood, the Pullmans, and Raymond Daudel, who, by and large, regarded the theory as too simplistic and extravagant.[20] In due course, however, Fukui’s theory was supported by Robert Mulliken’s work on the charge transfer theory and most importantly by the appearance of Woodward and Hoffmann’s paper on the conservation of orbital symmetry in 1965.[21] I will not go into detail about what followed, as these will be discussed by other speakers including Professors Buhm Soon Park and Noboru Hirota.

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[17] Kenichi Fukui, “The Role of Frontier Orbitals in Chemical Reactions,” Nobel Lecture, December 8, 1981, p.10. http://www.nobelprize.org/nobel_prizes/chemistry/laureates/1981/fukui-lecture.pdf

[18] Kosaku Kamio, “Fukui Kenichi sensei no omoide (My Memories of Professor Kenichi Fukui),” http://www.gijuturyoku.com/doc/doc11.html.

[19] Kenichi Fukui, Teijiro Yonezawa, and Haruo Shingu, “A Molecular Orbital Theory of Reactivity in Aromatic Hydrocarbons,” *Journal of Chemical Physics*, 20 (1952):722–725; Kenichi Fukui, Teijiro Yonezawa, Chikayoshi Nagata, and Haruo Shingu, “Molecular Orbital Theory of Orientation in Aromatic, Heteroaromatic, and Other Conjugated Molecules,” *Journal of Chemical Physics*, 22 (1954): 1433–1442.

[20] H. H. Greenwood, “Molecular Orbital Theory of Reactivity in Aromatic Hydrocarbons,” *Journal Chemical Physics*, 20 (1952): 1653; *idem*., “Some Comments on the Frontier Orbital Theory of the Reactions of Conjugated Molecules,” *ibid*., 23 (1955): 756–757; Kenichi Fukui, “A Simple Quantum-Theoretical Interpretation of the Chemical Reactivity of Organic Compounds,” in P.-O. Löwdin, B. Pullman eds., *Molecular Orbitals in Chemistry, Physics, and Biology* (New York: Academic Press, 1964), pp. 513–537.

[21] Robert S. Mulliken, “Molecular Compounds and their Spectra. II,” *Journal of the American Chemical Society*, 74(1952): 811–824; *idem*., “Molecular Compounds and Their Spectra. III. The Interaction of Electron Donors and Acceptors,” *Journal of Physical Chemistry*, 56 (1952): 801–822; R.B. Woodward and Roald Hoffmann, “Stereochemistry of Electrocyclic Reactions,” *Journal of the American Chemical Society*, 87 (1965): 395–397.

**Maintaining Theoretical Chemistry in an Applied Setting**

Kita died in 1952, and Kodama left Kyoto for Sumitomo Chemical Company in 1957. Now, Fukui was in a position to continue the academic tradition of his department. In 1966, the Department of Fuel Chemistry was renamed the Department of *sekiyu kagaku* which literally means petroleum chemistry. However, at Shingu's strong suggestion, the official English name was translated into the "Department of Hydrocarbon Chemistry." In the Faculty of Engineering, Fukui was tactful enough to maintain his circle of quantum chemistry in his *koza*. He managed a laboratory where his associate professor and assistants worked on conventional experimental studies on fuel-related practical subjects, such as catalysis, polymerization, and organic syntheses, while a select group of theoretical chemists focused on the expansion of his frontier orbital theory. That is to say that his *koza* consisted of two sections: experimental section and theoretical section.

Fukui, together with his coworkers, published 466 papers. Of these, about 60 % stemmed from the theoretical section, while the rest stemmed from the experimental section.[22] The experimental section filed nearly 200 patents with Fukui's name as one of the applicants. Through the experimental section, Fukui kept a good connection with industrial firms such as Sumitomo, which provided his *koza* with financial support. The study of the experimental section had nothing to do with quantum chemistry. Fukui needed the experimental section not to support or verify his frontier orbital theory, but to keep his theoretical section alive in a practical academic setting. That was a pragmatic way of *koza* management. He also encouraged his students to work first at the experimental section before entering the theoretical section, because he believed that theoretical chemists should have actual chemical experiences. As a number of quantum chemists and computational chemists emerged from the theoretical section, the Fukui school of theoretical chemistry flourished in Kyoto's Engineering Faculty.

**Conclusions**

In Fukui, we see the inquisitive mind of an experimental chemist, the intuitive faculty of a theoretician and mathematician, and the pragmatic mindset of an engineer. As Roald Hoffmann put it, "The building of a career in an applied setting was, I believe, crucial—it sensitized Fukui to problems of real chemical reactivity. In this he had an advantage over his 'purer' theoretician colleagues."[23] Fukui recalled that had he been a physicist in a physics department, he could not have done such a prize-winning work in quantum chemistry.[24] He acquainted himself with real chemical problems more than any theoretical physicists. Unlike many other applied chemists, he was well versed in mathematics and theoretical physics. Reciprocal intellectual stimuli between theoretical physics and chemical practices profoundly enhanced his scientific creativity.

Fukui succeeded in quantum chemistry because he stayed not in the Faculty of Science but in a strongly applied setting in the Engineering Faculty. Perhaps, Fukui was indeed materially better off in the Engineering Faculty than he might have been in the Science Faculty. Had he stayed at the Engineering Faculty in Tokyo University or somewhere else, he could not have done what he did at Kyoto. It was the unique tradition created by Kita and Kodama that nurtured him as a successful quantum chemist. How useful quantum chemistry was for fuel chemistry was not material to Fukui and his followers. Taking over that unique tradition, Kenichi Fukui skillfully founded a research school of quantum chemistry in Kyoto's Engineering Faculty in the 1960s.

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[22] Taken from SciFinder.
[23] Roald Hoffmann, "Obituary: Kenichi Fukui (1918–98)," *Nature*, 391 (19 February 1998): 750.
[24] Fukui, *Gakumon no sozo* (note 8), p. 114.