Obituary

Kenichi Fukui (1918–98)

Theoretical chemist who had fundamental insights into chemical reactivity

Kenichi Fukui, the first Japanese Nobel laureate in chemistry, died on 9 January this year. When Fukui was born, the electronic theory of chemical bonding was in its infancy. Oh, chemists did have a very well-grounded chemical notion of a bond and a symbolism for it. But the electron itself had barely reached maturity, and Lewis and Langmuir were just assimilating the then new Bohr quantum theory of the atom into chemistry.

By the time Fukui completed his education in 1941, things were different. The first textbook of quantum chemistry had been written six years before by a German in exile, Hans Hellmann. And American and British chemists had secured a place for quantum mechanics in chemistry, through the charismatic expositions of Linus Pauling, the quieter and deep reflections of Robert Mulliken, and the elegant, perceptive teaching of Charles Coulson.

Fukui wrote that chemistry was not his favourite subject in high school. His father (the family is an old Nara one), however, enquired of Gen-itsu Kita, a professor at Kyoto Imperial University, what his bright son might study. Kita suggested that Kenichi should enter the department of industrial chemistry. In those days children listened to the advice of their elders, and Fukui graduated from that department in 1941.

Some important work on synthetic aviation fuels during the Second World War led to an appointment in the department of fuel chemistry, in the faculty of engineering of Kyoto Imperial University. Much productive experimental work on reaction engineering and catalysis followed. 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. It is also an interesting counterpoint to the generally assumed inflexibility of Japanese universities and the *koza* system that Fukui could, in the end, do what elsewhere would be labelled as 'pure' chemistry in an applied setting.

For this young scientist had all along had theoretical aspirations and talents. He told me that he read Dirac's quantum theory text in the dull moments (I never found out if there were many or few)

between exploding American bombs. After the war, he gathered around himself a talented group of theoretical students, and in 1952 published in the *Journal of Chemical Physics* the paper that defined the idea of frontier orbitals.

Erich Hückel's seminal ideas on the stability of π-electron systems were finally receiving their due in just those years, and simple molecular orbital theory was in the ascendancy. Chemistry *is* reactivity; so it was natural to think of reducing the surfeit of information in the wavefunctions (how much worse it is now!) to a few pithy numbers, indicators of reactivity.

Various reactivity indices were devised, most emphasizing the charge distribution in the molecule as a whole. Fukui, Teijiro Yonezawa, Chikayoshi Nagata and Haruo Shingu's brilliant simplifying idea was to concentrate on one orbital — the highest occupied molecular orbital of the molecule when the reaction was with an acid; the lowest unoccupied molecular orbital when the reaction was with a base; and the singly occupied molecular orbital for a radical reaction. They called these orbitals the frontier orbitals of the molecule.

This notion, of tracing the essence of basicity or acidity or radical reactivity to a single orbital, was so simple! And, remarkably, it worked. The underpinnings of the idea were easily found by Fukui in perturbation theory, the natural language of quantum mechanics. In time, he and his co-workers expanded their ideas into a wide-ranging theory of orbital interactions and reactivity.

I first met Kenichi Fukui in early 1964. In the very next year our lives were inextricably bound together, when R. B. Woodward and I developed the concept of orbital symmetry control of organic reactions. Ours was a primitive frontier orbital approach, developed intuitively and graphically, and buttressed by simple molecular orbital calculations. Our idea of a controlling orbital was in the spirit of Fukui. And indeed Fukui could right away derive all of our conclusions. What happened next was interesting, in that the success of the orbital symmetry ideas very naturally heightened, retrospectively, the respect of the world community for Fukui's frontier orbitals.

For Kenichi Fukui and me, science for once worked the way it should on the human level — instead of a competition there developed a friendship. Part of our bond was formed by the four talented Fukui graduate students who then were postdocs with me. Kenichi and I were brought together not by the accident of shared external recognition, but by a real kinship in spirit — yes, across cultures, and respectful of the cultural differences that enrich life — and by a shared philosophical outlook and scientific style.

In time he and I were awarded the Nobel prize in chemistry. The event had more serious consequences for Kenichi than for me. In the United States the eye of the public is on rock stars, and Nobel prize winners are relatively many. So — thank God — we are left alone. In Japan, Fukui, as the country's first chemistry laureate, had a tremendous burden of committees, official obligations and public appearances. It was not easy for this shy intellectual gentleman of the old school to face his duty. But he did so, with style.

Kenichi Fukui was impelled by the truest desire to understand this world, and especially our dear chemistry. He strove to do so in pictures of conceptual simplicity and real depth. And he understood so well that the nature we have tried to comprehend (and what our creation has added to it) is a precious gift, unique, and worth preserving.

So I miss him, as does our chemical community. I remember our first encounter on Sanibel Island, precisely 34 years ago. And, among many subsequent meetings, one shared moment rises vividly — together we watched a great Kyoto ceramic master, Miyashita Zenju, his old hands trembling, then steadying as he put them on the clay turning on his wheel.

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