

Obituary

Kenichi Fukui: recollections of a friendship

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Early this year Prof. Kenichi Fukui, our friend, passed away. We are greatly saddened, and we offer condolences to Mrs. Tomoe Fukui and the children. Here, in turn we relate a few of our memories of Professor Fukui.

My teacher Bryce Crawford, the distinguished molecular spectroscopist, once said to me in graduate school, “In American physical chemistry, there was Gibbs and now there is Kirkwood”. I mention this remark because in thinking about Japanese post-World War II quantum chemistry, I conclude that one could well say that in Japanese quantum chemistry (as distinct from molecular spectroscopy), there was Kotani, and then there was Fukui. Of course Sugira [1] was the one who completed the Heitler–London treatment of the hydrogen molecule [quite a task to do even nowadays without the use of a canned computer program for computing molecular integrals!]. But it was Masao Kotani, a physicist, who began quantum-chemical research in the 1930s [2], and then for many years led the development in Japan of “ab initio” quantum chemistry in the modern sense of that term: compute everything correctly, and eschew unwarranted simplifications. I met Kotani at the Shelter Island Conference in late 1951 [3]. He soon sent me two postdoctoral workers, Teturo Inui and Tadashi Arai, and he once spent Christmas in our home. That is another story, but it sets the tone for this one. Physical science is a truly international discipline. A physical scientist moves in a world that has no national or other boundaries. Our community exemplifies how men and women from every place and every race can live and work together harmoniously.

It was with this orientation and this attitude, then, that I met and came to know Kenichi Fukui at a 1963 summer workshop on quantum chemistry in Constance, Germany, at which we both lectured. It was not that we talked a lot; it was just a certain companionship we both felt, the recognition that we were sharing the labor, the

fun, and the excitement of doing research in a difficult, fascinating, and important field. Later Professor Fukui and I met many times in many places. Hiroshi Nakatsuji and Akimoto Tachibana came to my laboratory from his as postdoctoral researchers. Fukui was responsible for several of the invitations I received to spend time in Japan. I am particularly grateful to him for having allowed me to serve as a trustee of the Institute of Fundamental Chemistry in Kyoto.

I had been fascinated with Fukui’s research well before I met him, from reading the works about frontier orbitals and the frontier theory of chemical reactivity [4], especially the pro and con arguments that appeared in the *Journal of Chemical Physics* [5]. I viewed the situation from a double-sided viewpoint that combined a commitment to the “ab initio” approach and a respect for the pre-World War II dogma that simple descriptions ought to be preferred. This led me to go out of my way to meet Alberte Pullman, Bernard Pullman, and Raymond Daudel, early in 1954, these three (among others) also being unafraid to venture into large-molecule chemical reactivity theory armed only with primitive quantum chemical tools. Subsequently I followed such problem areas as they were advanced through improvements of the ab initio methods themselves. Earlier ideas were never set aside, however, especially the frontier electron ideas.

It was in this context that in the late 1970s we began to work on the density functional theory of electronic structure. We soon found mutually supportive connections with the frontier ideas of Fukui. Density functional theory provided a scheme in which the electron density $\rho(r)$ takes the place of the wavefunction, and right in this scheme are quantities directly identifiable with electronegativity [6], hardness and softness [7, 8], and the frontier-electron concepts of Fukui [9–11]. If a molecule has nuclei that give rise to a potential $V(r)$ acting on N electrons and a total ground-state electronic energy $E[N, V]$, then

$$dE = \mu dN + \langle p dV \rangle \quad (1)$$

$$d\mu = \eta dN + \langle f dV \rangle \quad (2)$$

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where

$$\mu = \left(\frac{\partial E}{\partial N} \right)_V, \quad \eta = \left(\frac{\partial^2 E}{\partial N^2} \right)_V = \left(\frac{\partial \mu}{\partial N} \right)_V = \frac{1}{S} \quad (3)$$

and

$$f(r) = \left[\frac{\partial p(r)}{\partial N} \right]_V = \left[\frac{\delta \mu}{\delta V(r)} \right]_N. \quad (4)$$

Here μ is the negative of the electronegativity, η is the hardness, S is the softness, and $f(r)$ is what we chose to call the Fukui function as a token of our esteem for Professor Fukui. The name has stuck, and by now there is a lot about it in the literature. Since density functional theory is an exact theory, $f(r)$ is an accurate carrier of the original frontier orbital ideas. I believe that Professor Fukui welcomed these developments.

When people from different cultures become friends, there can be depths of understanding never reached, and aspects of personality that never come into play. So it was in the case of Kenichi Fukui and me. He must have chuckled inside when he beat me in a game of Go; I never asked him to play chess. More than once he befriended our son and his family, who lived in Japan.

When speaking at Professor Fukui's retirement party in Kyoto in 1982, I found myself on a podium beside which stood a magnificent, ancient, bonsai tree. For a moment I was speechless. I cannot forget that tree. At the end of the talk I proffered a verse (which was meant to be a paraphrase of frontier electron theory):

Theories come, and theories go
Simple wins; that's what we know
Orbitals, in full array
Hide essence, put off the day
Strip off those, that stay unblessed
Truth is there: in the few, the rest

Robert G. Parr

In the early spring of 1981, Bob and I enjoyed a visit from Kenichi and Tomoe Fukui to North Carolina. Sometime later Professor Fukui wrote a brief autobiography for the Nikkei newspaper. The story caught the attention of my former Japanese tutor, who sent me her translation of part of the article:

On my way back to Japan, I stopped at the University of North Carolina to give a lecture. My wife and I stayed at Professor Parr's home which is in a forest in Chapel Hill. Chapel Hill is a beautiful town where many American scholars choose to live after their retirement. Dr. and Mrs. Parr took us to a Chinese restaurant one evening. After dinner, I picked one of the fortune cookies, which said, "Stay still as firewood and that will fire your bigger desire." They asked me to show it to them, but I did not feel like showing it for some reason. I answered, "No, it is my secret." They laughed and said it must be something about romance.

Some days after we came back to Japan, I received a telegram from the US National Academy of Sciences informing me that I had been elected as a foreign associate of the Academy. It had been 19 years since I

had received Japanese Academy awards in 1962. I felt so happy, because it was an evaluation from abroad. This showed me friendship and good faith from Professor Parr and other friends who were members of the National Academy of Sciences. I wished now that I had shared the prophesy of the fortune cookie.

When the Fukuis arrived for this visit, they wore long faces and confessed to having a serious problem. It seemed that their daughter, Miyako, whom we had met as a little girl, was now grown up and well-educated, but unmarried and wanting to move out of the house. The trouble was that she would not let her mother arrange a marriage for her. Tomoe has been a go-between for many successful marriages. However, I recall during our first visit she had told me that she felt the future lay with the West, and while Professor Fukui was very traditional, as were his elderly parents, who lived with them, she was raising the children in a more Western manner. We met his parents whose living quarters were in a separate wing of the home. I will never forget the dignity of his father, who wore a black kimono as he showed us his most prized possession, an ancient Buddhist scroll. Tomoe managed to keep her husband and his parents content with proper recognition of the traditional ways, while at the same time instructing her son and daughter in modern ways. She had been so successful that the daughter now was causing concern!

Tomoe asked me, "What would an American mother do if her unmarried daughter wanted to move out of the home?" I laughingly replied, "I would help her pack." However, I went on to explain that there were many opportunities for young women today. I suggested that Miyako visit us in the summer. She could look into opportunities for graduate work, consult career counselors, and speak with our two daughters who were professionals. They thought this was a good idea, and said that they would relay our invitation to Miyako. A few weeks later, Miyako wrote me that her brother was going to take a special course at Brandeis University and that she was going to Boston to keep house for him and to take English lessons.

In October it was announced that Professor Fukui had won the Nobel prize, and the whole family was put in the national spotlight. There was much written for the press and many pictures and television interviews. As the result of this, one young man, the son of a famous professor of philosophy at Kyoto University, fell in love with Miyako! But how was he to meet her?

The Nobel prizes were awarded in Sweden in December. Miyako could not accompany her parents, because she had to stay home with her elderly grandparents. So while the festivities were going on abroad, the young man found a way to be introduced to her. It seems that the doctor who had attended her birth was the same one who had attended his. The doctor graciously supplied the proper introduction. The happy young couple saw one another often in a short time, and when the parents returned from Sweden, they announced that they were in love and wished to marry.

Needless to say, the next time we saw the Fukuis, they had happy faces. As Tomoe related the love story to me,

she positioned one hand horizontally, elbow-high, and said, “Chemistry professor – low echelon.” Then she took the other hand and put it above her head, saying, “Philosophy professor – high echelon.” Then she raised the lower hand to the position of the raised hand and said, “Nobel prize! High echelon!”. Thus a union had been realized, combining traditional elements with a more Western concept of love: a tribute to both parents!

The last time we dined with the Fukuis in Kyoto, Kenichi had phoned to ask our preference for a traditional or “other” meal. Knowing what a traditionalist he was, we chose traditional. Fukui and his driver picked us up at our hotel, and we were pleased to be driven to a restaurant we had enjoyed on previous visits. We left our shoes at the bottom of the stairs and walked up to meet Tomoe, who had arrived early in order to help set a Western table. Because of a back problem, she found it uncomfortable to sit on the floor, but she assured us that we would have a traditional Japanese meal. The evening was delightful. After dinner, we walked down the stairs, put shoes on, and went out amidst bows from the kimono-clad attendants. Kenichi, Bob, and I chatted in the narrow, cobbled street while we waited for Tomoe. It was the 15th of the month and the moon was full, which in Japan makes it a special moon. Someone suggested that the moon and the occasion demanded a haiku. Though none was composed, I was reminded of a haiku graciously given to us a few years earlier by Professor Fukui’s longtime colleague and collaborator Prof. Teiji Yonewawa. Yonezawa had dined with us in Chapel Hill on another beautiful moonlit evening. What he had written seemed to fit the Kyoto occasion as well:

Tsuki michi te	Full moon in the sky,
Ikoku no Utage	A dinner in a foreign land
Haten to su	is coming to an end.

Finally, Tomoe came out of the restaurant. She was wearing geta, which seemed strange. She approached me and said, softly, “Jane, I think you have my shoes on.” I did! Black pumps, size 7. They felt even better than mine!

We all laughed as we said goodbye. I did not know it would be my last goodbye to Professor Fukui.

Jane B. Parr

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