The Roles of Kenichi Fukui and Roald Hoffmann and R. B. Woodward in the Quantum Chemical Revolution

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The 20th century witnessed several revolutions in chemistry, one being the Quantum Chemical Revolution. In this lecture, the meaning of "revolutions in science" will be discussed and a working definition of this topic will be presented.[1] Specific and unique research contributions of Kenichi Fukui and Roald Hoffmann will be presented and evaluated for their unique contributions to the Quantum Chemical Revolution, a major conceptual and sociological leap in the discipline of chemistry. Beginning in the early 1950s, Professor Fukui invented the idea of frontier molecular orbitals (FMOs), the highest filled or electron-occupied MOs in a reacting center of one reactant interacting with the lowest energy unfilled MOs of a second reactant.[2] Fukui then applied perturbation theory (PT) with FMOs to explain chemical reactivity.[3] In 1964-1969, Hoffmann together with R. B. Woodward used a variety of quantum chemical tools including Hoffmann's very own independent derivation of FMO theory with PT, to derive the mechanisms of cyclic concerted reactions (electrocyclizations, cycloadditions, and sigmatropic reactions).[4] In 1981, Professors Fukui and Hoffmann shared the Nobel Prize in Chemistry for their seminal achievements, though at the time, there was no anticipation that a revolution in chemistry was in progress or their role in that revolution. (Woodward died in 1979 so he was ineligible for the 1981 Nobel Prize. Still, Woodward did receive the 1965 Nobel Prize in Chemistry.) Importantly, only a very few breakthroughs in science and certainly not all Nobel Prize-worthy accomplishments lead to revolutions in chemistry. The distinction between breakthrough science and the precipitation of a revolution in science will be highlighted. Kenichi Fukui and Roald Hoffmann together with R. B. Woodward achieved both.

1) J. I. Seeman, *J. Am. Chem. Soc. Au* **2023**, *3*, 2378-2401. 2) J. I. Seeman, *Chem. Rec.* **2022**, *22*, doi.org/10.1002/tcr.202100297; doi.org/10.1002/tcr.202100300; doi.org/10.1002/tcr.202100302. 3) K. Fukui, "A Simple Quantum-Theoretical Interpretation of the Chemical Reactivity of Organic Compounds" in *Molecular Orbitals in Chemistry, Physics, and Biology. A Tribute to R. S. Mulliken* (Eds.: P.-O. Löwdin, B. Pullman), Academic Press, New York, **1964**, pp. 513-537. 4) R. B. Woodward, R. Hoffmann, "The Conservation of Orbital Symmetry," *Angew. Chem. Int. Ed.* **1969**, *8*, 781-853, doi.org/10.1002/anie.196907811. See also: https://onlinelibrary.wiley.com/doi/toc/10.1002/(ISSN)1528-0691.woodward-hoffmann-rules