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Fukui K. Recognition of stereochemical paths by orbital interaction. *Account. Chem. Res.* 4:57-64, 1971.
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A practical, theoretical means, the HOMO-LUMO interaction method, based on the idea of the interaction of particular orbitals in the reacting molecules, is presented as an aid to understanding various stereochemical pathways occurring between molecules. This approach is a substitute for the Woodward-Hoffmann method using the principle of the conservation of orbital symmetry. [The *SCI*® indicates that this paper has been cited in over 335 publications.]

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This paper was written at the Illinois Institute of Technology, Chicago, where I stayed for half a year as a National Science Foundation senior Foreign Scientist Fellow. However, the basic idea for my HOMO-LUMO (highest occupied molecular orbital-lowest unoccupied molecular orbital) interaction scheme was born and developed earlier while I was in Kyoto; the idea was merely "rewarmed," so to speak, in Chicago.

I am embarrassed that this article has been selected as a *Citation Classic* because this is an instructive or explanatory article rather than an original paper. My intention was to reverse the unpopularity of my chemical reactivity theory presented in the majority of my papers. These papers were frequently criticized as having too many mathematical formulas, and in other cases, as containing some ambiguities. Thus my approach was not widely used by organic chemists. The Woodward-Hoffmann formulation was less mathematical, and its procedure was much more comprehensible to chemists. A *Physics Today* article covering the 1981 Nobel Prize in chemistry made this interesting statement: "One thinks of the analogous situation with the Feynman and Schwinger [both are 1965 Nobel Prize winners for physics] formulations of quantum electrodynamics."[1]

The frequent citation of this paper is perhaps due to its style, which does not look like my usual papers. The procedure described does not require any computation. Every organic chemist can do it; all that is required is elementary qualitative knowledge about the phase relationships of HOMO and LUMO of a few of the simplest species. On the other hand, even if the paper is not elaborate, I feel that it is complete. But before experimental chemists can apply the procedure, I think they must at least determine whether their experimental result can be treated as a one-step reaction.

Further, in order to use this approach, a more solid theoretical understanding is needed of the reaction path along which each of these procedures would be carried out. A theory of the reaction path was later developed,[2] and by using it, one can judge the likelihood of each path by purely theoretical calculation. In addition, the shape of interacting HOMO and LUMO changing along the reaction path can be calculated (theoretically) using equations presented by H. Fujimoto.[3] A. Koide also developed a method to present such a diagram using computer graphics.[4] Accordingly, one can, in principle, "visualize" the path of a chemical reaction by the orbital interaction approach.

The later developments of the HOMO-LUMO interaction scheme are comprehensively described by me in a more recent paper.[5]

1. **Schwarzschild B M.** Nobel Prize for chemistry to Fukui and Hoffmann. *Phys. Today* 34:20-2. 1981.
2. **Fukui K.** The path of chemical reactions—the IRC approach. *Account. Chem. Res.* 14:363-8. 1981.
3. **Fujimoto H, Koga N & Fukui K.** A coupled fragment molecular orbital method for interacting systems. *J. Amer. Chem. Soc.* 103:7452-547, 1981.
4. **Koide A, Doi A & Kajioka K.** Polyhedral approximation approach to molecular orbital graphics. *J. Mol. Graphics* 4:149-60. 1986.
5. **Fukui K.** Role of frontier orbitals in chemical reactions. *Science* 218:747-54. 1982.