

---

# Free Complement theory as an exact and general electronic structure theory

Hiroshi Nakatsuji\*

Quantum Chemistry Research Institute,

Kyoto Technoscience Center 16,14 Yoshida Kawaramachi, Sakyo-ku,

Kyoto 606-8305, Japan

[h.nakatsuji@qcri.or.jp](mailto:h.nakatsuji@qcri.or.jp)

---



## Abstract

Exact and general theory for solving the Schrödinger equation (SE) is a key for formulating an accurate predictive methodology in chemical science, since the SE is a governing principle of atoms, molecules, materials, and even biologies. Free complement (FC) theory is an exact general theory for solving the SE. It was published in 2004 after systematic studies on the structure of the exact wave function [1]. Because of its exact structure, this theory permits us to formulate different levels of theories that are useful for different purposes, but they altogether can be made exact. Each level of chemical concept is useful and the final exact concept is particularly useful for chemical studies. Since the basic concept in chemistry is local and transferable as seen in molecular structural formulas and chemical reaction formulas, which we refer to together as chemical formula, we present chemical formula theory (CFT) as a general variational molecular electronic structure theory. It describes the electronic structures of molecules in both ground and excited states, starting from the interactions of various atomic states to form molecules. Starting from CFT, we formulate the FC-CF variational theory, which is an advanced theory of CFT on the line of the FC theory using only the integratable complement functions ( $cf$ 's) of the FC-CF theory. Then, by further adding the effect of the non-integratable  $cf$ 's, we get the FC-CF exact theory. The wave functions of these theories are commonly featured by the local structure of the chemistry formulas. Therefore, they are useful not only for getting accurate energies and wave functions, but also the chemical concept of each level of the theory. In particular, the exact concepts obtained from the FC-CF exact theory will give the reliable understanding of the chemistry under study, which may give some inspirations to the chemists for further developing their chemistries, which may lead them to their successful goals. Here, some results [2] obtained along this line of the research will be presented.

---

## Reference and notes

[1] H. Nakatsuji, PRL 93, 030403 (2004); Acc. Chem. Res. 45, 1480 (2012).

[2] H. Nakatsuji, H. Nakashima, Y.I. Kurokawa, to be published.