Imperial Prize and Japan Academy Prize to:

Keiji Morokuma

Research Leader, Fukui Institute for
Fundamental Chemistry, Kyoto University
Professor Emeritus, Emory University, U.S.A.
Professor Emeritus, Institute for Molecular Science
Professor Emeritus, Graduate University for
Advanced Research

for "Theoretical Studies of Design of Structure, Function and Reactivity of Molecules"

Outline of the work:

In recent years the application of quantum theory to chemistry has accomplished high accuracy and, riding on the remarkable progress of new methodology and the availability of high performance computers, it has made a large transition from simple molecular systems to more complex and larger molecular systems. It is now reaching a new era of prosperity.

Dr. Morokuma has been playing the leading role in the development of this field as a successor of Dr. Kenichi Fukui's academic tradition and as an international leader in quantum molecular science. The research objectives of Dr. Morokuma's studies, in addition to the development of new powerful methodology, cover a wide range of molecular systems including large and complex molecular systems such as proteins. His research objectives can be divided into three major areas below and a few representative examples from each area will be presented in detail.

1. Theoretical studies of carbon nanostructures

Carbon nanostructures such as fullerenes and nanotubes have attracted much interest because of their novel structure and properties, and many studies have been performed on these structures. However no clear mechanism has been established on how small carbon species reach organized structures like fullerenes and nanotubes under high temperature conditions. Dr. Morokuma used a combined method of the electronic structure and molecular dynamics theories to study the mechanism of formation of fullerenes. He proposed the "hot shrinking giant fullerene" mechanism and attracted international attention; in the proposed mechanism self-assembly of small carbon species produces thermally excited giant fullerenes, which subsequently in the annealing process eject C_2 and other small species to reach C_{60} and other fullerenes.

2. Development of the energy gradient method and theoretical studies of design of chemical reactions

Dr. Morokuma developed energy gradient techniques as powerful tools for determination of reaction pathways and mechanisms of chemical reactions and applied them to complicated reaction systems including atmospheric and combustion reactions. These techniques made the analysis and design of chemical reactions as easy as solving "picture puzzles" and have been used very widely around the world. He used these methods himself and studied systematically the mechanism of reactions of homogeneous catalysis

by transition metal complexes. Such studies include the mechanism of the Wilkinson catalysis as well as polymerization and nitrogen activation catalysis. Furthermore he demonstrated that theoretical/computational approaches can predict functions of catalysts and are useful in designing new and more efficient catalysts. Such approaches of theoretical design of homogeneous catalysts have been adopted by chemical industries around the world and have contributed significantly to development of new catalysts including those for olefin polymerization.

3. Development of the ONIOM method and applications to complex molecular systems

Molecular systems that exhibit important chemical phenomena and properties are often giant molecular systems, and existing theoretical simulation methods had serious difficulties originating from the conflict between accuracy and computability. Dr. Morokuma developed the ONIOM method, a hybrid method in which a molecular system is divided into different regions and the most reliable method is used for the most important region where the origin of the function lies, whereas less reliable but easier methods are used for less important regions. This method is very flexible and has been used by many researchers world-wide for many different applications. Such applications include theoretical design of homogeneous and inhomogeneous catalysts, prediction of chemical properties of giant molecules that have never been synthesized, reaction design of highly selective organic synthesis, molecular and reaction design of nanoclusters, and relationship between the structure and reactivity of metalloenzymes. This method, a breakthrough for theoretical studies of large molecular systems, has been leading to new findings that had not been obtained by the existing methods and is expected to increase its importance in the future.

As described above, theoretical studies of Dr. Morokuma have lead the world for a long time, and he has received the Medal of the International Academy of Quantum Molecular Science, the Chemical Society of Japan Award, the Schrödinger Medal of The World Association of Theoretical Organic Chemists (WATOC), the Fukui Medal of Asian Pacific Association of Theoretical & Computational Chemists. He was also the President of the International Academy of Quantum Molecular Science, a world-wide organization of theoretical molecular science, for two terms.