Theoretical Studies of Chemical Reactions – Gas Phase Reactions to Nano Structures, Catalyses, and Enzymatic Reactions in Ground and Excited Electronic States

Keiji Morokuma

Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto 606-8103, Japan and Cherry L. Emerson Center for Scientific Computation and Department of Chemistry, Emory University, Atlanta, GA 30322, U.S.A.

The chemical reaction which creates, destroys, reorganizes chemical bonds to produce new compounds is the most important subject of chemistry. I have been absorbed by this exciting world of chemical reactions from the beginning of my career for more than fifty years, since a hand-powered calculator was used to solve Hückel secular equations for frontier electron densities of simple aromatic hydrocarbons. Theoretical/computational studies have come a long way and are now playing the central role in understanding the mechanism and dynamics of chemical reactions and in helping designing more useful chemical reactions and catalysts. The theory can study not only the reaction of the ground state of molecules in gas phase but also reactions of excited electronic states as well complicated reactions of complex molecular systems. The information theoretical/computational studies can provide is often complementary to the information experimental studies provide, and research on chemical reactions is becoming impossible without strong collaboration between theorists and experimentalists.

I will discuss a few examples of recent theoretical/computational studies performed in my group on chemical reactions. The areas to be covered include A. efficient and automatic determination of reaction pathways; B. self-assembly reactions of small carbon clusters to form fullerenes and carbon nanotubes with or without transition metal catalysts; C. homogeneous catalyses in solution and in the confined space created by protein, D. reactions of metalloenzymes with active site models and in protein environment, and E. chemical and biochemical processes involving excited electronic states.