NANYANG TECHNOLOGICAL UNIVERSITY

CBC SEMINAR ANNOUNCEMENT

Professor Keiji Morokuma
Kyoto University

Exciting World of Theoretical Studies of Chemical Reactions - From Gas Phase Reactions to Nano Structures, Catalysts, and Enzymatic Reactions

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 recent examples of our recent theoretical/computational studies on A. efficient determination of reaction pathways; B. the first excited-state "roaming" pathway for photodissociation of NO_3; C. self-assembly reactions of small carbon clusters to form fullerenes and carbon nanotubes; D. homogeneous catalysis, E. reactions of metalloenzymes in protein environment, and F. chemical processes involving excited electronic states of biomolecules.

Date:	**26th March 2012 (Monday)**
Time:	**2pm – 3.30pm**
Venue:	**NTU SPMS CBC Building Level 2, Conference Room**
Host:	**Asst Professor Hajime Hirao**