

Ústav fyzikální chemie J. Heyrovského, v.v.i.
Akademie věd České republiky

zve všechny zájemce na ústavní seminář,
na kterém promluví

Professor Keiji Morokuma

*(Fukui Institute for Fundamental Chemistry, Kyoto University;
Cherry L. Emerson Center for Scientific Computation and Department of
Chemistry, Emory University, Atlanta)*

na téma

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

Abstrakt:

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. self-assembly reactions of small carbon clusters to form fullerenes and carbon nanotubes; C. homogeneous catalysis, D. reactions of metalloenzymes in protein environment, and E. chemical processes involving excited electronic states of biomolecules.

Seminář se koná [v pátek 24. června 2011 od 14 hodin](#)

v Brdičkově posluchárně ústavu v Praze 8, Dolejškova 3.

Těšíme se na Vaši účast. Hosté jsou vítáni.

