CSO202A
Lec: MWTh: 12:00-12:50 L3
Tut: Fri: 17:00-17:50 T207-209

Module 1: Chemical Reaction Dynamics with Molecular Beams

This module is based on the molecular beam experiments for which Herschbach, Lee, and Polanyi received the **nobel prize in 1986**. Illustrate the key concepts using the F + D2 reaction as studied by Neuwark et al. J. Chem. Phys **82**, 3067 (1985). We will discuss, how one can visualize molecules in motion during a reaction through experiments.

Module 2: Ultrafast Reaction Dynamics with Lasers

Here the Ahmed Zewail's seminal work on femtochemistry will be discussed. His pioneering investigation of fundamental chemical reaction on ultrafast time-scale to captured the molecular birth have brought a revolution in chemistry and adjacent sciences. Focusing on the classic experiments on ICN (Dantus et al. *J. Chem. Phys.* **1987**, *87*, 2395) and NaI (Rose et al. *J. Chem. Phys.* **1988**, *88*, 6672) we will learn the technique that allows the monitoring of reactions on very short time scales - short enough to analyze transition states in selected chemical reactions. [**Nobel Prize in Chemistry, 1999**]

Module 3: Catalytic Reactions on Solid Surfaces

The aim of this module is to understand the molecular mechanism, role of catalyst and role of nitrogen molecule and atom in the Haber-Bosch process, based on the classic experiment of Gerhard Ertl (*Angew. Chem.* **1990**, *29*, 1219). We will discuss the concept and techniques to probe reaction on the surface. [**Nobel Prize in Chemistry, 2007**]

Module 4: Dynamics of Molecules with Supercomputers

We will discuss how to study structure and dynamics of molecules using extensive computations on supercomputers (up to million processors). This module will be based on two Nobel prize winning works. **Nobel prize in 1998** was awarded to John Pople and Walter Kohn for calculations of electronic structures of molecules. **Nobel prize in 2013** was given to Martin Karplus, Michael Levitt and Arieh Warshel for the development of computational models for computational modeling of complex chemical systems.

QUIZ-1: 27 th Jan. 2016
QUIZ-2: 31 st Mar. 2016
MIDSEM & ENDSEM : as per DOAA

* Assignments: a few assignments will be given, and the rest will be discussed during the tutorial hours. They don't have to be submitted.

* Mark distribution:
Quiz-1 (45 mins): 15% (module 1)
Quiz-2 (45 mins): 15% (module 3)
MidSem (2 hrs): 35% (module 1 + module 2)
EndSem (2 hrs) : 35% (module 3 + module 4)