课程名（Coursename）
Chemical Dynamics

课程代码（Coursenumber）
L5

课程对象（Audience）
Graduates

开课教师（Teacher）
Prof M. Sprik and Dr M. T. Cvitas

学期（Semester）

课程描述（Description）
The general objective of chemical dynamics is explaining the rates of chemical reactions in terms of a microscopic mechanism. More specifically, one aims to compute the rate starting from first principles classical or quantum mechanics. This is the subject of this course. The course is divided in two parts, chemical dynamics in the gas phase (SCA) and in solution (MS).
To predict a rate exactly one must calculate the wave function describing the motion of the atoms during the reaction. We explain the general nature of such wave functions and how they may be calculated accurately for simple gas-phase reactions. We then explain how to approximate this dynamics using Newtonian mechanics, or a combination of Newtonian and quantum mechanics, so as to include quantum tunnelling and zero point energy effects.
This leads us to a rigorous derivation of transition state theory, which provides a simple unifying explanation of many chemical reactions. We also discuss when transition state theory fails. The central concept in the solution chemistry part of the course is again transition state theory, how this theory can be derived for a condensed phase environment and how it can be used to understand solvent effects on reaction rates. We will also examine situations where transition theory breaks down and derive more general equations for reaction rates. The key theoretical tool for this part of the course is classical statistical mechanics. Quantum effects, although they can be important, will not be considered.
Topics Reaction dynamics: atomic motion on the femtosecond timescale. The wave functions of gas-phase reactions: introduction to quantum scattering theory. Classical theory of rates and classical transition state theory. Quantum corrections to transition state theory: the effect of tunnelling on reaction rates. When transition state theory fails. Some observations about reactions in solution relaxation and correlations in linear response theory. Transition state theory in the condensed phase, from potential energy surfaces to potentials of mean force. Diffusion, mobility and friction, Stokes Einstein relation. Marcus theory of electron transfer, non-equilibrium solvation and solvent reorganization.

课时信息（Totalhours）

教参信息（Textbookinfo）
1 Thermodynamics, Statistical Thermodynamics, & Kinetics (2nd Edition) by Thomas Engel and Philip Reid (Hardcover - Mar. 22, 2009)
ISBN-13: 978-0321615039
世界各地拥有馆藏的图书馆（OCLC）:66
2 Physical Chemistry for the Biological Sciences (Methods of Biochemical Analysis) by Gordon G. Hammes (Hardcover - Apr. 10, 2007)
ISBN-13: 978-0470122020
世界各地拥有馆藏的图书馆（OCLC）:322
3 Oxoacidity: reactions of oxo-compounds in ionic solvents (Comprehensive Chemical Kinetics) by Victor L. Cherginets (Hardcover - June 23, 2005)
ISBN-13: 978-0444517821
世界各地拥有馆藏的图书馆（OCLC）:120
4 Thermodynamics and Kinetics for the Biological Sciences by Gordon G. Hammes (Paperback - June 16, 2000)
ISBN-13: 978-0471374916
5 Statistical Thermodynamics: Fundamentals and Applications by Normand M. Laurendeau (Hardcover - Nov. 21, 2005)
ISBN-13: 978-0521846356
世界各地拥有馆藏的图书馆（OCLC）:172
6 Statistical Mechanics by Donald A. McQuarrie (Hardcover - May 2000)
ISBN-13: 978-1891389153
7 Thermodynamics, Statistical Thermodynamics, & Kinetics (2nd Edition) by Thomas Engel and Philip Reid (Hardcover - Mar. 22, 2009)
ISBN-13: 978-0321615039
世界各地拥有馆藏的图书馆（OCLC）:66
8 An Introduction to Thermodynamics and Statistical Mechanics by Keith S. Stowe (Hardcover - June 11, 2007)
ISBN-13: 978-0521865579
世界各地拥有馆藏的图书馆（OCLC）:170
9 Equilibrium and Non-Equilibrium Statistical Thermodynamics by Michel Le Bellac, Fabrice Mortessagne, and G. George Batrouni (Hardcover - May 3, 2004)
ISBN-13: 978-0521821438
世界各地拥有馆藏的图书馆（OCLC）:223
10 Thermodynamics and Statistical Mechanics (Classical Theoretical Physics) by Walter Greiner, Ludwig Neise, Horst Stöcker, and D. Rischke (Paperback - May 9, 1995)
ISBN-13: 978-0387942995
11 Introduction to Modern Statistical Mechanics by David Chandler (Paperback - Sept. 17, 1987)
ISBN-13: 978-0195042771