课程大纲
COURSE SYLLABUS

1.	**课程代码/名称** **Course Code/Title**	CHE5037/化学动力学和动态学
2.	**课程性质** **Compulsory/Elective**	专业课
3.	**课程学分/学时** **Course Credit/Hours**	2.00/32
4.	**授课语言** **Teaching Language**	英文
5.	**授课教师** **Instructor(s)**	姜洪岩
6.	**先修要求** **Pre-requisites**	物理化学 I

7. 教学目标
Course Objectives

Chemical kinetics and dynamics remains one of the most exciting areas in modern chemistry. A student that successfully completes this course will develop skills in methods that allow the quantitative description of chemical change. While many portions of the undergraduate chemistry curriculum emphasize descriptive and qualitative treatments, the present course develops a much more mathematical and computational formulation. Students will learn to construct predictive models that describe the time evolutions of chemical concentrations and other attributes of kinetic systems including ab initio theories of rate coefficients. In addition, this class emphasizes traditional mass action kinetics and statistical rate theories as well as molecular dynamics with emphasis on modern physical chemistry methods for examining molecular processes.

8. 教学方法
Teaching Methods

A student completing this course will learn to (1) compute the rates of chemical reactions using ab initio data using statistical theories of reaction, transition state theory and RRKM theory, (2) analyse the behaviour of complex reaction networks using methods such as sensitivity analysis, (3) construct kinetic models to represent problems of interest in physical chemistry and catalysis, (4) role of molecular beam and laser technologies in researching the processes of energy transfer, chemical reaction, and photodissociation. The course will not emphasize the mathematical treatment of collisions. Instead, the students will learn a more physically oriented view that allows the outcome of various processes to be predicted using simple models.

9. 教学内容
Course Contents

Section 1	Mass action kinetics. The construction of rate laws for elementary reactions in gas phase systems is discussed. The structure of kinetic equations for multi-step chemical mechanisms is presented including the role of conservation laws and micro-reversibility. Approximate solutions of the kinetic equations using the quasi-steady state approximation is presented. Network analysis and sensitivity analysis is discussed for complex mechanisms. Models for chain branching chemical reactions are presented. (4 credit hours)
Section 2	Evaluation of rate coefficients. Transition State Theory is derived for bimolecular chemical reactions. A brief review of statistical thermodynamics, kinetic theory of gases, and potential energy surfaces is presented as a necessary introduction to the formalism. Additional topics of discussion include the theory of quantum tunnelling, isotope effects, and thermodynamics formulation. (4 credit hours)

	Section 3	Unimolecular reactions and energy transfer. The RRKM theory of unimolecular reaction rates is derived. The role of intramolecular and intermolecular energy transfer is discussed. State counting algorithms are introduced. (4 credit hours)
	Section 4	Reactions in condensed phase environments. The theory of diffusion controlled reactions is presented for chemical reactions occurring in solution phase. Chemical reactions on catalytic surfaces is analysed. The rates of electron transfer reactions in condensed phase is modelled using the Marcus theory of electron transfer. (4 credit hours)
	Section 5	Molecular Collision: Molecular collisions in the gas phase are introduced. The idea of the collision cross section is used to describe chemical reaction and energy transfer. The connection to rate coefficients is stated. (2 credit hours)
	Section 6	Energy Transfer: Vibration. Vibrational energy relaxation in gas and condensed phase is discussed. The role of vibrational energy transfer in a gas phase environment is discussed. The single collision environment of molecular beam is also discussed. (2 credit hours)
	Section 7	Energy Transfer: Electronic. The quenching of electronically excited states is analyzed using simple theories such as the Landau-Teller molecule. (2 credit hours)
	Section 8	Dynamical of Chemical Reactions: The properties of chemically reactive molecular collisions are discussed. The connection between reactive cross sections and reaction rate coefficients is given. The role vibrational energy in promoting the reaction is analyzed using Polanyi's rules. (4 credit hours)
	Section 9	Molecular Beam Experiments: Modern experimental results involving crossed molecular beams are reviewed. The state of present experimental capabilities is discussed. The influence of reactant excitation and "reactive resonances" are shown. (4 credit hours)
	Section 10	Photodissociation Dynamics: The basic photochemical process of photodissociation is presented. The angular and state distribution of the products is show to reveal interesting aspects of the dynamical process. The intramolecular dynamics of molecules is shown to strongly influence the spectrum and decay dynamics of highly excited molecules. (2 credit hours)
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10.	**课程考核** **Course Assessment**
	出勤与课堂表现：20%；作业：30%；期末考试（开卷）：50%。
11.	**教材及其它参考资料** **Textbook and Supplementary Readings**
	Chemical Kinetics and Dynamics, by JI Steinfeld, JS Francisco, and WL Hase