南方科技大学 SOUTHERN UNIVERSITY OF SCIENCE AND TECHNOLOGY

课程详述

COURSE SPECIFICATION

以下课程信息可能根据实际授课需要或在课程检讨之后产生变动。如对课程有任何疑问，请联系授课教师。

The course information as follows may be subject to change, either during the session because of unforeseen circumstances, or following review of the course at the end of the session. Queries about the course should be directed to the course instructor.

1.	课程名称 **Course Title**	化学动力学和动态学 I **Chemical Kinetics and Dynamics Part 1**
2.	授课院系 **Originating Department**	化学系 Department of Chemistry
3.	课程编号 **Course Code**	CH328
4.	课程学分 **Credit Value**	1
5.	课程类别 **Course Type**	专业选修课 Major Elective Courses
6.	授课学期 **Semester**	春季 Spring
7.	授课语言 **Teaching Language**	英文 English
8.	授课教师、所属学系、联系方式（如属团队授课，请列明其他授课教师）**Instructor(s), Affiliation& Contact**（**For team teaching, please list all instructors**）	Professor Rex Skodje (a visiting professor of CHEM; a full professor from University of Colorado Boulder, https://www.colorado.edu/chembio/rex-t-skodje).
9.	实验员/助教、所属学系、联系方式 **Tutor/TA(s), Contact**	无 NA
10.	选课人数限额(可不填) **Maximum Enrolment**（**Optional**）	

11\. 授课方式 **Delivery Method**

	讲授 **Lectures**	习题/辅导/讨论 **Tutorials**	实验/实习 **Lab/Practical**	其它(请具体注明) **Other（Please specify）**	总学时 **Total**
学时数 **Credit Hours**	16				16

12.	先修课程、其它学习要求 **Pre-requisites or Other Academic Requirements**	物理化学 I（CH301）
13.	后续课程、其它学习规划 **Courses for which this course is a pre-requisite**	
14.	其它要求修读本课程的学系 **Cross-listing Dept.**	

教学大纲及教学日历 SYLLABUS

15. 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.

16. 预达学习成果 **Learning Outcomes**

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, and (3) construct kinetic models to represent problems of interest in physical chemistry and catalysis

17. 课程内容及教学日历 （如授课语言以英文为主，则课程内容介绍可以用英文；如团队教学或模块教学，教学日历须注明主讲人）
Course Contents (in Parts/Chapters/Sections/Weeks. Please notify name of instructor for course section(s), if this is a team teaching or module course.)

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 hrs)

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 hrs)

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 hrs)

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 hrs)

18. 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

课程评估 ASSESSMENT

19.

评估形式 **Type of Assessment**	评估时间 **Time**	占考试总成绩百分比 **% of final score**	违纪处罚 **Penalty**	备注 **Notes**
出勤 **Attendance**		0		
课堂表现 **Class Performance**		10		
小测验 **Quiz**		20		
课程项目 **Projects**		0		
平时作业 **Assignments**		20		
期中考试 **Mid-Term Test**		50		
期末考试 **Final Exam**		0		
期末报告 **Final Presentation**		0		
其它（可根据需要改写以上评估方式） **Others (The above may be modified as necessary)**		0		

20. **记分方式 GRADING SYSTEM**

☑ A. 十三级等级制 **Letter Grading**
☐ B. 二级记分制（通过/不通过） **Pass/Fail Grading**

课程审批 REVIEW AND APPROVAL

21. 本课程设置已经过以下责任人/委员会审议通过
This Course has been approved by the following person or committee of authority

化学系教学指导委员会
Teaching committee of the chemistry department