

# CH 421 & L: Chemical Dynamics

School of Engineering and Science

# **Fall 2022**

Instructor: Dr. Rahul L. Khade

Contact Info: Office: EAS 410; rkhade@stevens.edu;

TAs: Maxine Zhao: xzhao55@stevens.edu; and Thompson Hui, thui@stevens.edu

Class Meeting Times: Lecture: Monday/Wednesday/Friday 10:00-10:50 AM;

Lab: Monday 2:00-5:50PM/Tuesday 11:00AM-2:50PM (McLean 516)

Lecture session: EAS 329

Office Hours Hybrid: Wednesday 2-3 PM. In person in office EAS 410 or via zoom Meeting ID: 930

2343 6293. (https://stevens.zoom.us/meeting/93023436293) Appointments via

email are needed for efficient management.

Prerequisites: CH 321 or E 234; MA 221 or MA 281.

Corequisites: None Cross-listed with: None

#### COURSE DESCRIPTION

This is one of the most challenging chemistry courses. This course provides the physical basis for indepth understanding of chemistry, particularly the theories and applications of chemical dynamic processes. The objective of this course is to let students grasp some basic concepts and laws involved in chemical dynamics, and to develop the skills of how to use theoretical concepts and methods to understand chemical properties and processes that are governed by physical chemistry laws. A number of approaches will be employed to help students learn some fundamental principles and also the techniques to solve problems in these areas, so that students' physical understanding of chemical dynamic processes and related quantitative skills will be greatly enhanced. Upon completing the course, students will be able to solve some problems in these areas and to write and speak about chemical dynamics and related topics in Physical Chemistry.

# STUDENT LEARNING OUTCOMES

#### After successful completion of this course, students will be able to...

- 1) Use gas kinetic theory to calculate characteristic speeds: most probable speed, average speed, and root-mean-square speed, and mean free path
- 2) Calculate gas diffusion coefficient and viscosity
- 3) Determine reaction order, rate constant, and the integrated rate law from the differential rate law
- 4) Calculate the half-life for the elementary chemical reaction
- 5) Apply the pre-equilibrium approximation, steady-state approximation, and mass conservation to derive relationships in a multi-step reaction
- 6) Calculate partial molar quantities and colligative properties
- 7) Express mean ionic chemical potential, mean ionic activity, mean ionic activity coefficient in terms of individual ions' chemical potentials, activities, and activity coefficients, and use Debye-Hückle theory to calculate mean ionic activity coefficient

8) Calculate cell potentials for electrochemical reactions and use Nernst equation to calculate thermodynamic properties.

# COURSE FORMAT AND STRUCTURE

This course is fully in-person. To access the course, please visit <u>stevens.edu/canvas</u>. For more information about course access or support, contact the TRAC by calling 201-380-6599 or 201-216-5500.

# **Course Logistics**

Our weeks will run from Monday to Sunday. All times mentioned in this class are defined as Eastern Time (as used in Hoboken, NJ).

Deadlines are an unavoidable part of being a professional and this course is no exception. Course requirements must be completed and posted or submitted on or before specified due date and delivery time deadline. The specific due date and time information is in syllabus and Canvas. If there is no specific due time, then the due time is 11:59 PM of the due date.

# **Instructor's Office Hours (Hybrid)**

I will be available in-person in EAS 410 or via zoom (link provided on page 1) for office hours Wednesday 2-3 PM. Other times you can contact me via email and will respond as soon as I am available (generally within 24-48, except for weekend/holiday) hours. When emailing me, please place in the subject line the course number/section and the topic of the email (i.e. CH 421 – Homework 2 Question). This will help me tremendously in locating your emails quicker because I receive numerous emails each day.

# **Class Etiquette Guidelines**

Your instructor and fellow students wish to foster a safe in-class learning environment. All opinions and experiences, no matter how different or controversial they may be perceived, must be respected in the tolerant spirit of academic discourse. You are encouraged to comment, question, or critique an idea but you are not to attack an individual. Our differences, some of which are outlined in the University's inclusion statement below, will add richness to this learning experience. Working as a community of learners, we can build a polite and respectful course ambience. Please read the following:

- Give other students the opportunity to join in the discussion.
- Do not use offensive language. Present ideas appropriately.
- Keep an open mind and be willing to express even your minority opinion.
- Do not hesitate to ask for feedback.

#### **COURSE MATERIALS**

**Textbook:** Physical Chemistry, 11th Edition, by Peter Atkins and Julio De Paula,

Oxford, 2018

**Materials:** Scientific calculator

# **COURSE REQUIREMENTS**

**Attendance** To help students understand physical chemistry concepts, theories, and problems, and

master essential problem-solving skills, class attendance is mandatory for every student. An excused absence will require documentation, such as a note from a doctor or

clearance in advance (e.g. for a professional interview).

Participation 1) To promote active learning, the instructor will ask questions in each class. A student

will earn a bonus of 2 points for every academic question answered correctly by

himself/herself (not by reading textbook or other materials or using other resources) or by

a group in which he/she is a member, in the class. This student needs to write down the question and the answer, emailed to instructor with subject of "CH 421: Bonus question" at the end of the class, as an evidence, except that the questions are asked in the lecture slides and thus answers have already been collected by certain software (such as Poll Everywhere). 2) A student is expected to bring LAPTOP/smart phone (for Polleverywhere participation) to the class, as some questions need calculations and/or Stevens owned software or web search, will be deliver using Canvas and quizzes/exams on Paper. 3) If a student has a useful and workable suggestion for the class that is accepted by the instructor, he or she will get 10 points for such a suggestion. These total bonus points x10% will be the bonus in the final grade.

#### Homework

Homework problems help students understand the contents lectured in the class. In addition, the homework problems are chosen to train students with better skills critical to solve important physical chemistry problems, for which similar problems may appear in the exams to ensure students grasp the essential concepts and techniques. In this way, they aid students to improve research skills and prepare for passing exams with better grades. As shown in the following table, there are five sections of topics, and for each section there is a homework assignment and it is due one week after that section is done. No late homework is accepted, except for medical emergency, death in immediate family, or other serious cause, for which the written documentation and approval of the professor are required. Homework answers must be hand-written and submitted to the professor via a scanned copy. Homework assignments will be graded on the basis of completion (if one problem is solved in detail to the final answer, it will get full credit). Each base homework grade equals to 100 points x (No. of problems solved/ No. of problems assigned). Students are highly recommended to do additional problems to improve problem-solving skills. Each additional problem solved can earn 5 extra points in that homework grade, with a cap of total 50 extra points for one homework. The overall homework grade in the final grade is calculated as total points/5 x 10%. The homework shall follow the following format:

- 1) first line: write your full name, CH421 Homework No. x (*x* is the actual section No. from 1-5 for the submitted homework)
- 2) write "Required": for each problem, first write the problem No. (no need to copy problem), then give full solution.
- 3) write "Bonus" (if one wants to do extra problems for bonus credit: for each problem, first write the problem No. (no need to copy problem), then give full solution.

Homework No.	Section	Focus	Homework from Textbook	Due Date
1	Molecular	1/16	Focus 1B:	9/21/2022
	Motion		Exercises: 1a) 2a) 5a) 6a) 7a)	
			Focus 16A:	
			Exercises: 2a) 7a) 8a)	
2	Basic Reaction	17/18	Focus 17A:	10/3/2022
	Kinetics		Exercises: 2a) 3a) 5a) 7a) 9a)	
			Focus 17B:	
			Exercises: 3a) 5a) 6a)	
			Focus 17D:	
			Exercises: 1a) 2a) 3a)	
3	Complex	17	Focus 17E:	10/31/2022

	Reaction		Exercises: 1a) 2a) Problems: 5 & 9	
	Kinetics		Focus 17F:	
			Exercises: 4a) 5a)	
			Focus 17G:	
			Exercises: 3a) Problems: 7	
4	Solution	5	Focus 5A:	11/16/2022
	Properties		Exercises: 8a) 9a) 10a) 11a)	
			Focus 5B:	
			Exercises: 2a) 3a) 5a)	
			Focus 5F:	
			Exercises: 1a) 2a) 5a) 7a)	
5	Electrochemical	6	Focus 6C:	11/30/2022
	Reaction		Exercises: 1a) 2a) 3a) 4a)	
			Focus 6D:	
			Exercises: 1a) 2a) 3a) Problems 1 & 5	

# **Quizzes**

After each section is finished, a quiz will be given one week later. So, it is on the same day of the section homework due date as described above. The quiz usually takes <10 min to finish, but the first 15 min of a class session is given for a quiz if needed. If someone is late, the time will not be extended. Quizzes will be graded for accuracy. If a student has any question about the quizzes, s/he can make an appointment with the professor to go over them before the final exam. Each quiz grade equals to 100 points x No. of problems solved correctly/ No. of problems assigned. If a student is absent (unexcused) on a day that a quiz is given s/he will receive an automatic zero for that quiz. Should a student have to miss a quiz because of medical emergency, death in immediate family, or other serious cause, written documentation and approval of the professor are required. The overall quiz grade in the final grade is calculated as total quiz points/ total No. of graded quizzes x 10%.

#### **Exams**

There are three exams. The student can only use a scientific non-programmable calculator in the exam. If one is discovered to cheat in an exam, s/he will get an F in the final grade. Topics covered for each exam are listed in the end of this syllabus. Generally, there are no makeup exams. Should a student have to miss an exam because of medical emergency, death in immediate family, or other serious cause, written documentation and approval of the professor are required. In such a case, if this student can have a time that is within one week after the exam date and is also convenient for the professor, it may be made up. Otherwise, the final grade will be determined by appropriately weighted average by removing this missed exam grade. Missing any exam without an excuse approved by the professor will result in a zero grade for that exam.

# Labs

To help students understand more of some concepts and skills in the Chemical Dynamics area and gain additional hands-on experience of some Chemical Dynamics experiments, there is a lab section. Additional materials including experimental details, demonstrations, reports, grading policy, and schedule for this lab section will be distributed by TA. Students will be generally put in groups of two (although a slightly larger group like three might occur depending on situations). To further expand the learning and practice experience, a student may work on an experiment that the relevant theory has not been lectured yet, and some experiments may not correspond to the specific theories in the lecture series in this semester. However, the full theoretical background along with all experimental details plus demonstrations will be provided, in addition to personal helps from TA should any questions arise. Moreover, a three-week work period will be given for each experiment: one week lab time for the lab itself, second week lab time for report preparation along with questions and discussion with TA,

and the report work can be continued and is due by the third week lab day for submission (and start of next lab experiment). This is another kind of guided learning to enrich the education experience, and further prepare a student for future independent and teamwork.

#### **Paper**

This paper project will allow you to demonstrate your understanding and knowledge of chemical dynamics to real world applications in a topic of your personal interest. Choose AT LEAST three peer-reviewed journal articles pertaining to your research topic (each should be cited in appropriate places of the paper) and you will describe how the chemical dynamics concept/principle were applied to this topic. The paper shall have at least 1,000 words. The file name shall have the format as FirstnameLastname-ProjectPaper.docx. All pages need to be numbered and use times new roman, 12 point, double-space, normal margins, portrait, and letter size settings. Each paper shall begin with a project title, then student name, and the following three sections with the section titles shown here: A) **Introduction:** Describe which chemical dynamics concept/principle will be covered in this paper, why this topic area is important and what kinds of specific problems are to be solved using this concept/principle; B) Results and **Discussion**: Describe in detail with examples of literature data and figures to show how the selected chemical dynamics concept/principle help solve some specific problems to advance science; C) Conclusion: Describe briefly the main idea of the selected chemical dynamics concepts/principles, and the main conclusions of using such concepts/principles to help solve real-world problems. D) **References**: put the cited references here, using the format as in the most cited chemical journal, Journal of the American Chemical Society. The full grade in this section is 100, which is 10% of final grade and due on 12/12/2022. If someone misses one section or the cited references/data/figures do not support the chemical dynamics concept/principle, 10 points will be deducted. If someone has one of the following mistakes, 5 points will be deducted for each mistake: a) no data table; b) no figure; c) less than 3 peer-reviewed journal articles cited; d) missing one or more required descriptions in sections A-D as mentioned above. If someone has one typo or grammatical error or format error, each of such errors costs 1 point.

**Presentation** You will give a short 15-minute presentation with group of 2 in last week of the class on the topic you picked for the paper. The schedule of the presentations will be determined in the class.

# **TECHNOLOGY REQUIREMENTS**

# Baseline technical skills necessary for online courses

- Basic computer and web-browsing skills
- **Navigating Canvas**
- Laptops/smart phones for PollEverywhere (PollEverywhere is free)

# **Required Equipment**

- Computer: current Mac (OS X) or PC (Windows 7+) with high-speed internet connection
- Calculators

# **Required Software**

- Current or first previous major release of Chrome, Firefox, Edge, or Safari browser
- Microsoft Word, Excel, PowerPoint

#### GRADING PROCEDURES

#### Grades will be based on:

Class Participation	(5 %)
Homework	(10 %+bonus)
Quizzes	(5 %)
Paper-Presentation	(10 %)
Exam I	(15 %)
Exam II	(15 %)
Final Exam	(15 %)
Lab	(25 %)
Total	100%+(~5%)bonus

#### **GRADING SCALE:**

A	100%	to	93%
A-	< 93%	to	90%
B+	< 90%	to	87%
В	< 87%	to	83%
B-	< 83%	to	80%
C+	< 80%	to	77%
C	< 77%	to	73%
C-	< 73%	to	70%
D+	< 70%	to	67%
D	< 67%	to	60%
F	< 60%	to	0%

# **ACADEMIC INTEGRITY**

# **Undergraduate Honor System**

Enrollment into the undergraduate class of Stevens Institute of Technology signifies a student's commitment to the Honor System. Accordingly, the provisions of the Stevens Honor System apply to all undergraduate students in coursework and Honor Board proceedings. It is the responsibility of each student to become acquainted with and to uphold the ideals set forth in the <u>Honor System Constitution</u>. More information about the Honor System including the constitution, bylaws, investigative procedures, and the penalty matrix can be found online at http://web.stevens.edu/honor/

The following pledge shall be written in full and signed by every student on all submitted work (including, but not limited to, homework, projects, lab reports, code, quizzes and exams) that is assigned by the course instructor. No work shall be graded unless the pledge is written in full and signed.

# **Reporting Honor System Violations**

Students who believe a violation of the Honor System has been committed should report it within ten business days of the suspected violation. Students have the option to remain anonymous and can report violations online at www.stevens.edu/honor.

#### **EXAM ROOM CONDITIONS**

The following procedures apply to quizzes and exams for this course. As the instructor, I reserve the right to modify any conditions set forth below by printing revised Exam Room Conditions on the quiz or exam.

<sup>&</sup>quot;I pledge my honor that I have abided by the Stevens Honor System."

1. Students may use the following devices during quizzes and exams. Any electronic devices that are not mentioned in the list below are <u>not</u> permitted.

Device	Permitted?		
Device	Yes	No	
Laptops		X	
Cell Phones		X	
Tablets		X	
Smart Watches		X	
Google Glass		X	
Other (Nonprogrammable calculator)	X		

2. Students may use the following materials during exams. Any materials that are not mentioned in the list below are <u>not</u> permitted.

Material		Permitted?	
		No	
Handwritten Notes		X	
One page Notes and formula sheet (to be submitted with exam)	X		
Textbooks		X	
Readings		X	

3. Students are not allowed to work with or talk to other students during quizzes and/or exams.

#### LEARNING ACCOMODATIONS

Stevens Institute of Technology is dedicated to providing appropriate accommodations to students with documented disabilities. The Office of Disability Services (ODS) works with undergraduate and graduate students with learning disabilities, attention deficit-hyperactivity disorders, physical disabilities, sensory impairments, psychiatric disorders, and other such disabilities in order to help students achieve their academic and personal potential. They facilitate equal access to the educational programs and opportunities offered at Stevens and coordinate reasonable accommodations for eligible students. These services are designed to encourage independence and self-advocacy with support from the ODS staff. The ODS staff will facilitate the provision of accommodations on a case-by-case basis.

For more information about Disability Services and the process to receive accommodations, visit <a href="https://www.stevens.edu/office-disability-services">https://www.stevens.edu/office-disability-services</a> (Links to an external site.). If you have any questions please contact: Phillip Gehman, the Director of Disability Services Coordinator at Stevens Institute of Technology at pgehman@stevens.edu or by phone 201-216-3748.

#### **Disability Services Confidentiality Policy**

Student Disability Files are kept separate from academic files and are stored in a secure location within the Office of Disability Services. The Family Educational Rights Privacy Act (FERPA, 20 U.S.C. 1232g; 34CFR, Part 99) regulates disclosure of disability documentation and records maintained by Stevens Disability Services. According to this act, prior written consent by the student is required before our Disability Services office may release disability documentation or records to anyone. An exception is made in unusual circumstances, such as the case of health and safety emergencies.

#### INCLUSIVITY

# Name and Pronoun Usage

As this course includes group work and class discussion, it is vitally important for us to create an educational environment of inclusion and mutual respect. This includes the ability for all students to have their chosen gender pronoun(s) and chosen name affirmed. If the class roster does not align with your name and/or pronouns, please inform the instructor of the necessary changes.

#### **Inclusion Statement**

Stevens Institute of Technology believes that diversity and inclusiveness are essential to excellence in academic discourse and innovation. In this class, the perspective of people of all races, ethnicities, gender expressions and gender identities, religions, sexual orientations, disabilities, socioeconomic backgrounds, and nationalities will be respected and viewed as a resource and benefit throughout the semester. Suggestions to further diversify class materials and assignments are encouraged. If any course meetings conflict with your religious events, please do not hesitate to reach out to your instructor to make alternative arrangements.

You are expected to treat your instructor and all other participants in the course with courtesy and respect. Disrespectful conduct and harassing statements will not be tolerated and may result in disciplinary actions.

#### MENTAL HEALTH RESOURCES

Part of being successful in the classroom involves a focus on your whole self, including your mental health. While you are at Stevens, there are many resources to promote and support mental health. The Office of Counseling and Psychological Services (CAPS) offers free and confidential services to all enrolled students who are struggling to cope with personal issues (e.g., difficulty adjusting to college or trouble managing stress) or psychological difficulties (e.g., anxiety and depression). CAPS is open daily from 9:00 am – 5:00 pm M-F. Evening hours are available by appointment in the Fall / Spring semesters and up-to-date information regarding the availability of evening appointments can be found by visiting <a href="https://www.stevens.edu/CAPS">www.stevens.edu/CAPS</a> (Links to an external site.). To schedule an appointment, call 201-216-5177.

Due to the pandemic, in-person appointments may be limited until further notice. Up-to-date information about the availability of in-person services can be found at <a href="www.stevens.edu/CAPS">www.stevens.edu/CAPS</a> (Links to an external site.). Teletherapy (therapy via secure video platform) is available to registered students physically located in the states of New York or New Jersey. Students located outside of NY / NJ are encouraged to pursue local treatment through their personal health insurance. To learn more about the process of finding a therapist please visit the CAPS webpage on <a href="Seeking Help Off-Campus">Seeking Help Off-Campus</a> (Links to an external site.).

#### **EMERGENCY INFORMATION**

In the event of an urgent or emergent concern about the safety of yourself or someone else in the Stevens community, please immediately call the Stevens Campus Police at 201-216-5105 or on their emergency line at 201-216-3911. These phone lines are staffed 24/7, year-round. For students who do not reside near the campus and require emergency support, please contact your local emergency response providers at 911 or via your local police precinct. Other 24/7 national resources for students dealing with mental health crises include the National Suicide Prevention Lifeline (1-800-273-8255) and the Crisis Text Line (text "Home" to 741-741). If you are concerned about the wellbeing of another Stevens student, and the matter is *not* urgent or time sensitive, please email the CARE Team at <a href="mailto:care@stevens.edu">care@stevens.edu</a>. A member of the CARE Team will respond to your concern as soon as possible.

#### TENTATIVE EXAM SCHEDULE

Any and all changes to this schedule will be communicated to you 1) in class and 2) via email.

Date	Topic(s)
October 5	Exam 1: 10:00pm-10:50pm
November 2	Exam 2: 10:00pm-10:50pm
December 14	Final exam: 10:00pm-10:50pm

# EXAM REVIEW TOPICS

Exam	Section	Focus	Topics
1 <sup>st</sup>	Molecular	1B	Kinetic model's three assumptions
	Motion		Kinetic model's perfect gas law
			V <sub>mean</sub> , V <sub>mp</sub> , V <sub>rms</sub> , mean free path
		16A	Diffusion coefficient, Viscosity coefficient, their relationship
	Basic	17A	Reaction rate definition and calc (from reaction formula)
	Reaction		Rate constant unit and relationship with overall order; individual
			reactant order
	Kinetics	17B	For 0-2 order reactions, differential rate laws, to integrated rate
			laws, half lives
		17D	Arrhenius equation
		18C	Transition state theory concept
2nd	Complex	17C/E	Reversible reaction, consecutive reaction, parallel reaction
	Reaction		Pre-equilibrium, steady-state, mass conservation
	Kinetics	17F	Michaelis-Menton equation, Lineweaver-Burk equation,
			noninhibition & competitive inhibition
			$V_{max}$ , $Km$ , $k_{cat}$ , $\eta$
		17G	Photophysical processes
			Fluorescence and quenching
			Fluorescence resonance energy transfer
Final	Solution	5A	Raoult's law, Henry's law
	Properties	5B	Elevation of boiling point and depression of freezing point
			Osmosis
		5F	solvent activity
			mean ionic chemical potential, mean ionic activity, mean ionic
			activity coefficient
			use Debye-Hückle theory to calculate mean ionic activity
			coefficient
	Electrochemical	6C	Cell notation; half reaction
	Reaction	6C/D	Cell potential, standard potential
		6D	Use Nernst equation to calculate Thermodynamic properties