Syllabus for CHEM447601: Physical Chemistry II (Spring Semester, 2022)

Class schedule: Tuesday, Thursday, 10:30 AM to 11:45 AM **Location:** Merkert 130

Course website: https://www.lucasbaogroup.com/chem-course-2

(I post the course syllabus and problem sets online. The reading material (McQuarrie), solutions to the problem sets and midterm exams may be posted on *Canvas*.)

Recitation: All students must register for recitation/discussion session (Monday, 6 PM; **Campion 204**)!

Instructor: Prof. Lucas Bao (email: lucas.bao@bc.edu)

Office hours:

- Tuesday, 1:00 – 3:00 PM (Merkert 224)
- Thursday, 3:00 – 5:00 PM (Merkert 224)
- Friday, 4:30 – 6:00 PM (Merkert 224)

TA: Mr. Boqiang Chen (email: chenalr@bc.edu)

Recitation & Office hours:

- Monday, 6:00 – 7:00 PM: Recitation/Discussion session Location: Campion Hall, 204
- Tuesday, 2:00 – 4:00 PM (Merkert 030A)
- Wednesday, 12:45 – 2:45 PM (Merkert 030A)

Pre/co-requisites: CHEM4475 Physical Chemistry I, PHYS2201 Introductory Physics II
Highly recommended by not required: MATH2210 Linear Algebra (can be studied by active learning or taken concurrently through this course) and PHYS3100 Vibrations and Waves

Description and scope of the course: This course intends to build a foundation for understanding the structures of matter and chemical reactions *via* quantum mechanics and the relationship between structures and macroscopic properties *via* statistical mechanics. This course serves as the gateway to appreciating modern chemical science with rigorous and quantitative physical models. The topics to be covered include basic principles of quantum mechanics, exactly solvable systems, variational principle, molecular orbital theory and Hückel theory, Boltzmann distribution, ideal-gas statistical thermodynamics, and transition-state theory for reaction rate. **This course has three components: In-class lectures, recitations, and active learning (self-learning).**

Expectation. PChem II (Quantum & Statistical Mechanics) is an intense and challenging course (probably *the most* challenging chemistry course in your whole undergraduate training), which requires hard work, patience, self-discipline, and perseverance. In addition, please review your multivariable calculus! We have already tried to **only** include the **basic topics** that are of general interest for the understanding of reaction mechanisms, structure-property relations, and various spectroscopic measurements. We tried to reduce unnecessarily (to the level of the students, not to PChem itself as a subject) complex mathematical details as well. Nevertheless, it is unlikely that you will master the course material if you *only* go through it *once* during my lectures. (This is generally the case for a college-level class focusing on hard-core science.) However, our goal is to help you meet the **basic** requirements of the ACS standards (or, to some of you, the requirements for scoring high in the GRE subject test) and be better positioned for advanced learning (e.g., undergraduate research, graduate school).

How do we help you learn?

- **Communication channel**: Recitations, office hours, and email.
- **Dynamic feedback collection**: Email the TA about any topics that you struggled with the most, and we will go through them either in recitations, office hours, or in class.
- **Automatically recorded lectures**: Recorded videos will be available on Canvas ("Panopto Recordings"). However, the automatic lecture capturing system might not work so well, so it may miss part of the lecture or some of my notes on the blackboard.

Textbooks (required):

1. Peter Atkins and Julio de Paula, *Physical Chemistry* (The <u>9th</u> edition)

Comment: You may also find it helpful to use the **Solution Manual** to accompany the textbook. Other editions (e.g., from the 7^{th} to the latest version) also work if you cannot find the 9^{th} ed. (Almost the same content with slightly different organization.)

2. D. A. McQuarrie, *Mathematical Methods for Scientists and Engineers*

(I may post part of this textbook on *Canvas* as reading material in case you do not have access to full chapters.)

Comment: This textbook covers all the math needed to understand the course material. It is a user-friendly math textbook written by a physical chemist. We will assign math problems from this book, which require **self-learning** (or, **active learning**). The math topics that you must know (by studying this book) in this course include multivariable calculus (including doing integrals in three dimensions using polar coordinates), rudimentary linear algebra (determinant, matrix, eigenvalue and eigenvector), simple ordinary differential equations, and the basics of complex numbers.

References (optional):

1. Ira N. Levine, *Quantum Chemistry* (The Seventh edition)

Comment: An amazingly detailed and chemist-friendly introduction to basic quantum mechanics and its connection to chemistry.

2. P. A. M. Dirac, *The Principles of Quantum Mechanics* (The Fourth edition)

Comment: This bible is written by one of the founding fathers of quantum mechanics.

3. D. A. McQuarrie and J. D. Simon, *Molecular Thermodynamics*

Comment: Learn classical thermodynamics in a bottom-up approach, starting from the quantized energy levels in molecules and basic principles of statistical mechanics.

Written exams and grading:

- Exam 1 (Date: 02/22): In-class, closed-note/closed-book, 75-min test — 100 points
- Exam 2 (Date: 03/29): In-class, closed-note/closed-book, 75-min test — 100 points
- Exam 3 (Date: 04/26): In-class, closed-note/closed-book, 75-min test — 100 points
- Final exam (Date: 05/13): In-class (Merkert), open-note†/closed-book, 4-hour test — 150 points
- Problem sets (Due date: Refer to course outline on page 5) — 500 points

†Allow ***two double-sided*** letter pages of handwritten notes; nothing else is allowed, no textbook, no lecture notes!

Final score X

$$X = 40 \times \frac{(\text{Exam 1} + \text{Exam 2} + \text{Exam 3})}{3 \times 100} + 45 \times \frac{\text{Final Exam}}{150} + 15 \times \frac{\text{Problem Sets}}{5 \times 100}$$

Final course grade: Your final letter grade is the higher one between <u>grade 1</u> and <u>grade 2</u>, as determined below.

<u>Grade 1</u>: **A**: $X \geq 85$; **A–**: $85 > X \geq 80$; **B+**: $80 > X \geq 75$; **B**: $75 > X \geq 70$; **B–**: $70 > X \geq 65$; **C+**: $65 > X \geq 60$;
C: $60 > X \geq 55$; **C–**: $55 > X \geq 50$; **D+**: $50 > X \geq 45$; **D**: $45 > X \geq 40$; **D–**: $40 > X \geq 30$; **F**: $X < 30$.

<u>Grade 2</u>: $Z = (X - \text{class average})/\text{class standard deviation}$

A: $Z \geq 1.000$; **A–**: $1.000 > Z \geq 0.700$; **B+**: $0.700 > Z \geq 0.333$; **B**: $0.333 > Z \geq 0$;
B–: $0 > Z \geq -0.333$; **C+**: $-0.333 > Z \geq -0.666$; **C**: $-0.666 > Z \geq -1.000$;
C–: $-1.000 > Z \geq -1.333$; **D+**: $-1.333 > Z \geq -1.666$; **D**: $-1.666 > Z \geq -2.000$;
D–: $-2.000 > Z \geq -2.333$; **F**: $Z < -2.333$.

Please mark the exam date and the due date on your calendar.

The 75-min midterm exams (i.e., exams 1, 2, and 3) usually include four questions, one of which is a big-picture question that tests your conceptual understandings and does not require any detailed derivations or numerical calculations. In principle, one should be able to finish all questions within 1 hour (if you studied lecture notes and problem sets carefully and did the homework; by "studied", I meant that you tried to understand or reproduce what's covered, rather than like reading a novel and having a vague impression about where to find the concept). Nevertheless, I provide additional time to you to be flexible. You are not allowed to use any notes or textbooks during the midterms. The 4-hour final exam may include 8 long questions. (One should be able to finish all questions within 3 hours. Nevertheless, I will give you one more hour.) For the long questions, you must show all of your work for full credits. You are allowed to bring handwritten notes (*not exceeding two double-sided letter pages*) for the final exam. Nontrivial and complicated formulas and mathematical results may be provided in the questions when necessary.

The final exam is scheduled for the final exam week, from **12:30 PM** to **4:30 PM**. **The final exam is an open-note/closed-book exam.** You are allowed to use the handwritten notes (***not exceeding two double-sided letter pages***) during the **4-hour final exam**. Other resources (lecture notes, textbooks, laptops, etc.) are NOT allowed. All exams emphasize your fundamental understandings of the course material rather than challenging your mathematical skills; however, testing a certain amount of your mathematical ability cannot be avoided. Mastering essential mathematical techniques is indispensable in physical chemistry.

Homework: Homework (HW) includes **two parts**: **(a) reading assignments** and **(b) PChem problem set** (from Atkins and/or McQuarrie, plus additional questions that emphasize the material covered in class). In the lectures, I sometimes skip some of the details in the derivations. It is your responsibility to fill these gaps with the help of the reading material. In addition, it is critical to learn the basic mathematical background from McQuarrie's book (i.e., active learning – a must-have skill for your future career). PSs usually contain selected questions in the textbooks and may include additional questions that are designed to be pedagogical (and perhaps, challenging to some students); in other words, you can learn a lot (including some important topics that I did not cover in the lectures) by working out these questions in the PSs. The solutions will be posted on *Canvas*. TA will only grade a subset of the questions so that we can return your written solutions ASAP.

You are highly encouraged to discuss the problem sets (or the solutions to some questions, which are available in the solution manual) with us by using the communication channel. In addition, feel free to email us (the course TA and/or me) any questions you have about the course material or relevant background knowledge. Different students come in with different backgrounds. Everybody may advance in understanding at a different rate. That is expected. You are highly encouraged to work on PSs *before* you consult the Solution Manual. If you choose to work with your classmates, please make sure you write up your own solution. Please note that since the solutions to the majority of problems can be found in the Solution Manual, PSs will only be counted as 15% of your final score. However, this does not mean that you should not spend a significant amount of your effort on solving problems. **If you do not practice problem-solving**, you won't be able to test your understanding of the course material, and **you are highly likely to have a difficult time when taking the exam**. This is especially true in physical chemistry.

The due date of each PS is listed in the course outline. The PSs are collected at the beginning of the in-class discussion sessions. **Start these well ahead of their due dates as they require a substantial time investment to complete** (on average, *at least* ~ 6–8 hours every week).

The course TA will go through the problem sets (including both the math background and the PChem components)**, midterm exams, and review course material** (including math background) **in the recitation sessions and office hours.** It is highly unlikely (and unrealistic) for the TA to go through every question in the recitation sessions, and thus, you should go to TA's office hour (or schedule meetings with the TA), discuss problems with your classmates (form a study group!), and use the solution manual (and the solution posted on

Canvas) wisely.

For any physical chemistry course, **the key to understanding and mastering the course material is to practice on problems**. Before working on problems, you should review the lecture notes and read textbooks carefully, and more importantly, try to repeat the derivations *without* referring to these references. You are highly recommended (but not obligated) to study *all* the exercises and problems in your textbooks with the help of the Solution manual. Please contact the course TA regarding any concerns about the grading of your homework or exams.

Academic Integrity Policies: Please refer to https://www.bc.edu/bc-web/academics/sites/university-catalog/policies-procedures.html#academic_integrity_policies for a statement about the importance of academic integrity and a reference to the university's academic integrity policy.

Course outline:

Date	#Lecture	Topics [a]	Assignment
Tue 01/18	**1**	Course introduction The failure of classical description of matter	**Problem Set 1 (PS1: Lec 1-3)** Reading: Atkins,[1] Chapter 7; McQuarrie,[2] Chapter 4 & Chapter 11
Thurs 01/20	**2**	Wave-particle duality Bohr's hydrogen model Stationary states and standing waves on a ring	
Tue 01/25	**3**	Math review (Complex numbers & ODEs); Classical waves and vibrations; Separation of variables; Standing waves in a 1D box	Reading: McQuarrie, Chapter 21 (section 21.1 – 21.2)
Thurs 01/27	**4**	Time-independent Schrödinger equation; Probability descriptions and wavefunctions (well-behaved wavefunctions, orthornormalization)	
Tue 02/01 (Due: PS1) [b]	**5**	Time-dependent Schrödinger equation; Operators; Eigenvalue; Superposition	**Problem Set 2 (PS2: Lec 4-6)**
Thurs 02/03	**6**	Dirac notation; Hermitian operators;	
Tue 02/08		Continue lecture 6: Commutators; Uncertainty principle; Superposition	
Thurs 02/10	**7**	Free-particle wavefunctions; Particle in 1D box	Reading: Atkins, Chapter 8; McQuarrie, Chapter 12
Tue 02/15	**8**	Review: Expectation values for particle in 1D box; separation of variables (particle in 2D box); uncertainty principle	
Thurs 02/17 (Due: PS2) [b]	**9**	Introduction to important exactly solvable problems – Particle on a ring and microwave spectroscopy of diatomic molecules	**Problem Set 3 (PS3: Lec 7-13)**
Tue 02/22	**Midterm exam 1 (closed-book/closed-note, 75-min test)** **(10:30 AM – 11:45 AM Location: In class)** You will be tested on the material covered in lectures **1**–**8**.		
Thurs 02/24	**10**	1D Harmonic oscillator, zero-point energy, kinetic isotope effect, and IR spectroscopy	
Tue 03/01	**11**	Introduction to important exactly solvable problems – 1D tunneling & chemical kinetics	Reading: McQuarrie, Chapter 14 (sections 14.1–14.4)
Thurs 03/03	**12**	Hydrogen atom –Working with Schrodinger equation in 3D; Separation of variables; Wavefunctions, orbitals, quantum numbers	Reading: Atkins, Chapter 9; McQuarrie, Chapter 8 & Chapter 16 (section 16.6)
Tue 03/08 & Thurs 03/10	**No Class (Spring Break)**		
Tue 03/15	**13**	Introduction to angular momentum; Electron spin	Reading: McQuarrie, Chapter 9 (9.1–9.3) & 10 (10.2, 10.3, 10.5)

[a] Depending on the actual progress, we may cover less or (unlikely) more topics.
[b] The problem set (PS) is collected at the beginning of the lecture. Alternatively, you could schedule a meeting with the course TA to hand in your PSs. However, we do not accept works after due dates. If you choose to email your PS to us, please make sure you send it as a single PDF file with your name on it.

---

[1] Peter Atkins and Julio de Paula, Physical Chemistry (The 9th edition).
[2] D. A. McQuarrie, Mathematical Methods for Scientists and Engineers

Date	#Lecture	Topics [a]	Assignment
Thurs 03/17	**14**	Introduction to multielectron atoms; Slater determinant; Atomic term symbol	Reading: McQuarrie, Chapter 9 (9.1–9.3) & 10 (10.2, 10.3, 10.5)
Tue 03/22 (Due: PS3) [b]	**15**	Variational principle; Linear variation: Concept of molecular orbitals	**Problem Set 4 (PS4: Lec 14-18)** Reading: Atkins, Chapter 10
Thurs 03/24	**16**	Born-Oppenheimer approximation; The nature of chemical bond: The quantum mechanics of H_2^+ and H_2 (based on Linus Pauling's seminal works: *Chem. Rev*. 1928, 5, 173)	Reading assignment: (a) YouTube video – A conversation with Linus Pauling (Two-time Nobel Prize laureate): https://www.youtube.com/watch?v=a8maetlPd8Q (b) Linus Pauling's understanding of the nature of chemical bond: *Chem. Rev*. 1928, 5, 173. (Posted on the course website.)
Tue 03/29	**Midterm exam 2 (closed-book/closed-note, 75-min test)** **(10:30 AM – 11:45 AM Location: In class)** You will be tested on the material covered in lectures **9**–**15** primarily, but the course material covered in the previous lectures cannot be avoided in the test.		
Thurs 03/31	**17**	Introduction to rudimentary linear algebra; QM eigenvalue problem; Hückel theory for molecules	Reading: McQuarrie, Chapter 9 (9.1–9.3) & 10 (10.2, 10.3, 10.5)
Tue 04/05	**18**	Review & Problem Solving – H_2^+; Hückel method; H_2 molecule: from MO to VB (if time permits)	
Thurs 04/07	**19**	Basics of statistical thermodynamics – Microstates and microcanonical ensemble	Reading: Atkins, Chapter 15; McQuarrie, Chapter 21 (section 21.1)
Tue 04/12 (Due: PS4) [b]	**20**	Basics of statistical thermodynamics – Boltzmann distribution and canonical-ensemble partition function	**Problem Set 5 (PS6: Lec 19-23)**
Thurs 04/14 & Tue 04/19	**No Class (Eastern Weekend, Holy Thursday)** **&** **No Class (Substitute Monday Class Schedule)**		
Thurs 04/21	**21**	Basics of statistical thermodynamics – Ideal-gas thermodynamics	Reading: Atkins, Chapter 16
Tue 04/26	**Midterm exam 3 (closed-book/closed-note, 75-min test)** **(10:30 AM – 11:45 AM Location: In class)** You will be tested on the material covered in lectures **16**–**20** primarily, but the course material covered in the previous lectures cannot be avoided in the test.		
Thurs 04/28	**22**	Review & Problem solving – Ideal gas and heat capacity of solids (if time permits)	
Tue 05/03	**23**	Basics of statistical thermodynamics – From quantum mechanics to chemical reaction rates (Transition-state theory)	Reading: Atkins, Chapter 22
Thurs 05/05 (Due: PS5) [b]	**24**	• Wrap-up of previous lectures; • Special topics (~ 45min): From black-body radiation to quantum chemistry and quantum information; • Course Review (If time permits)	
Friday, 05/13 (12:30 PM – 4:30 PM)	**Final exam (closed-book/open-note, 4-hour test)** **Friday, 12:30 PM – 4:30 PM; Location: In class (Merkert 130)** Allow ***two double-sided*** letter pages of handwritten notes; nothing else is allowed, no textbook, no lecture notes! You will be tested on the material covered in lectures **1–23**. (Lecture 24 – "Special topics" is not part of the final exam.)		

[a] Depending on the actual progress, we may cover less or (unlikely) more topics.
[b] The problem set (PS) is collected at the beginning of the lecture. Alternatively, you could schedule a meeting with the course TA to hand in your PSs. However, we do not accept works after due dates.

Physical Chemistry Supplement

Context

Physical chemistry provides the fundamental concepts and organizing principles that underlie all aspects of chemistry and related fields. It develops rigorous and detailed explanations of central, unifying concepts in chemistry and contains mathematical models that provide quantitative predictions. Physical chemistry contains the mathematical underpinning to concepts applied in analytical, inorganic, organic, and biochemistry courses, as well as more advanced topics in chemistry. Physical chemistry techniques and explanations are used for atomic, molecular, nanoscale, mesoscale, and macroscopic materials.

Conceptual Topics

Physical chemistry should emphasize the connection between microscopic models and macroscopic phenomena and the transition from atomic scale to macroscopic scale materials, from both a theoretical and an experimental perspective. Courses should develop both qualitative and quantitative models of physical properties and chemical change, and students should critically apply these models to deepen their understanding of chemical phenomena. Problem solving is a key activity in learning physical chemistry. Physical chemistry courses typically require at least two semesters of calculus and two semesters of physics. Previous experience with multivariable techniques is highly desirable, and exposure to differential equations and linear algebra is very useful as well. In addition, prior chemistry courses may provide preparation for the principal areas of coverage in physical chemistry.

The core treatment of physical chemistry will typically address each of the major concepts listed in bold below. However, a two-semester course cannot cover all of the topics listed for each concept, and a one-semester course will require an even more judicious choice of topics and coverage. A broad survey of the concepts and in-depth treatment of selected topics is a common and effective approach. Because physical chemistry concepts underlie the descriptions of many phenomena, it is especially useful to include examples of current scientific interest, make connections to others areas in chemistry, and study interdisciplinary applications of physical chemistry.

- **Thermodynamics and equilibria**. Standard functions (enthalpy, entropy, Gibbs energy, etc.) and applications. Microscopic point of view especially for entropy. Chemical potential applied to chemical and phase equilibria. Non-ideal systems; standard states; activities; Debye-Huckel limiting law. Gibbs phase rule; phase equilibria; single and multi-component phase diagrams. Thermodynamics of electrochemical cells. Thermodynamics of elastomers and coil-type molecules.

- **Chemical kinetics.** Differential and integral expressions with emphasis on single-step and multi—stepphenomena of various orders. Relaxation processes. Microscopic reversibility. Derivation of rate laws from chemical mechanisms. Steady-state approximation. Chain reactions and polymerization. Collision theory; absolute rate theory; transition state theory. Isotope effect. Enzyme kinetics. Molecular reaction dynamics including molecular beams, trajectories, and lasers. Reactions on surfaces. Photochemistry.

- **Quantum mechanics**. Postulates and formulation of Schrodinger equations. Operators and matrix elements. Particle-in-a-box. Simple harmonic oscillator. Rigid rotor; angular momentum. Hydrogen atom; hydrogenic wave functions. Spin; Pauli principle. Approximate methods. Helium atom. Hydrogen molecule ion; hydrogen molecule, Diatomic molecules. LCAO method. Computational chemistry. Quantum chemistry applications.

- **Spectroscopy** (often interspersed with quantum mechanics to provide immediate applications). Light-matter interaction; dipole selection rules. Rotational spectra of linear molecules. Vibrational spectra. Term symbols. Electronic spectra of atoms and molecules. Magnetic spectroscopy. Raman spectroscopy; multiphoton selection rules. Lasers.

- **Statistical thermodynamics** (often associated with thermodynamics). Ensembles. Maxwell-Boltzmann distributions. Standard thermodynamic functions expressed in partition functions. Partition function expressions for atoms, rigid rotors, harmonic oscillators. Einstein crystal; Debye crystal.

- **Interdisciplinary applications**. Atmospheric, biophysical, materials, and/or quantum chemistry.

Practical Topics

The physical chemistry laboratory gives students experience in connecting quantitative models with observed chemical phenomena using physical chemistry concepts. The pedagogical goal is for students to understand the qualitative assumptions and limitations of models and the quantitative ability of the models to predict observed chemical phenomena.

Students must understand how to record good measurements, decide whether their measurements are valid, and estimate the errors in their primary experimental variables. This entails understanding the principles and use of electronic instrumentation for making measurements, as well as developing laboratory problem-solving experience with these instruments. Hands-on experience with modern instrumentation for measurement of physical properties and chemical change is essential. The opportunity for students to design aspects of their own experiments is quite valuable in learning about making measurements. During their data analysis, students must develop the ability to propagate experimental measurement uncertainties into uncertainties in calculated chemical quantities. A detailed error analysis is an important feature of physical chemistry laboratory reports.

Computers should assist in the collection, analysis, and graphing of data, as well as in the writing of reports. It is important that students gain experience with spreadsheet programs and linear least-squares fitting for data analysis. Computational tools such as Mathematica, MATLAB, or Mathcad are useful for helping students connect models to observed phenomena, and experiments using modern computational techniques (quantum calculations, molecular modeling) play an important role.

A sample list follows from which a set of experiments in physical chemistry might be selected. Within the physical chemistry area itself, as well as in an integrated laboratory, it is common for individual experiments to combine several aspects of experimental methods and theoretical concepts.

- **Thermodynamics.** Heat of combustion; enthalpy of reaction in solution. Thermodynamic functions from the temperature dependence of an equilibrium constant or the emf. Study of a system in which activity coefficients play a prominent role. Synthesis and characterization of solid state or polymeric materials.

- **Phase Equilibria**. Solid-liquid phase diagram. Liquid-vapor phase diagram.

- **Kinetic Theory**. Thermal conductivity of gases. Diffusion in solution. Knudsen effusion. Viscosity of gases.

- **Kinetics.** Relaxation study (first-order kinetics), possibly using lasers. Kinetic analysis of a complex reaction. Enzyme study.

- **Computational chemistry.** Molecular orbital theory. Calculation of structure and spectral properties

- **Spectroscopy.** Analysis of a vibration-rotation spectrum; isotope effects, e.g., HCl/DCl. Analysis of a polyatomic vibrational spectrum, e.g., SO_2. Analysis of an electronic-vibration spectrum, e.g., I_2. Analysis of electronic spectra, e.g., conjugated polyene dyes. Atomic spectroscopy. Raman spectroscopy. NMR analysis of spin-spin coupling in a non-first-order case. Laser applications.

- **Other.** Micelle formation

Illustrative Modes of Coverage

A common and traditional approach for teaching physical chemistry is a two-semester lecture and laboratory course taught in the third year. The laboratory program may accompany the lectures, be a separate course, or be an intensive single-semester course. The physical chemistry laboratory experience may also be integrated into a broader laboratory experience. These examples are not proscriptive, and creativity in the pedagogy and teaching of physical chemistry concepts is encouraged.

A one-semester course provides both opportunities and challenges for introducing students to the topics of physical chemistry within the context of a degree track. Often these courses provide a broad survey of the concepts and in-depth treatment of selected topics. The challenge of designing a one-semester course in physical chemistry is to determine the important principles that govern the physical and chemical behavior of matter within the context of the course emphasis. For example, a one-semester class for students who are pursuing a biochemistry track might focus on quantum chemistry, thermodynamics, and kinetics with examples from biochemistry used to illustrate these concepts. An environmental degree track could use examples based on analyzing field measurements or the kinetics of air pollutants.

Given the amount of material and time constraints of a one-semester class, some of the important topics in physical chemistry could be moved into other courses. For example discussions of enzyme kinetics could be incorporated into a course in biochemistry, kinetic modeling into an in-depth course in atmospheric chemistry, molecular orbital theory into physical organic or physical inorganic chemistry, and non-ideal solutions and electrochemistry into analytical chemistry. The choice of topics and coverage is at the discretion of the instructor and department; and discussion is encouraged within the department to ensure that important topics are not overlooked.

Independent of the focus of a one-semester physical chemistry course, students should be exposed to both microscopic and macroscopic aspects of physical chemistry, the relationship between these two approaches, and the use of quantitative models for understanding and predicting chemical phenomena of both large and small molecules. Discussion within and among departments is encouraged as the chemistry community works to develop one-semester physical chemistry courses that provide students with the necessary background and training to pursue a career in the chemical sciences.

Last revised in March 2015