

CHEM 260 – Advanced Physical Chemistry
Fall 2022 Syllabus

Instructor: Prof. Michael T. Ruggiero, Ph.D. (he/him)

Office: Innovation 342

Email: Michael.Ruggiero@uvm.edu

Office Hours: By appointment (just email me!)

Course Information

3 Credits

Class: TR 8:30-9:45

Location: Perkins 107

Required Text: *Physical Chemistry – A Molecular Approach*, Donald A. McQuarrie and John D. Simon. University Science Books, California. ISBN: 978-0-935702-99-6.

Recommended Reading: *Quantum – Einstein, Bohr, and the Great Debate About the Nature of Reality*, Manjit Kumar, W. W. Norton & Company.

Course Description and Goals

In this course you will learn the fundamental concepts that govern much of the chemical world that you have explored thus far. The beauty of physical chemistry lies in the underpinning mathematics that elegantly describe atomic level phenomena, and without a doubt this course will explore these concepts in detail. This course aims to delve deeper into the quantum mechanical and thermodynamic areas that you have previously explored, but with much more mathematical rigor. Building from the ground up, you will quickly see how a few lines of calculus is sufficient to describe complex observables, and will be able to recognize the fundamental origins of the world around you. The learning objectives are simple: by the end of this course you should feel equipped to be able to describe chemical systems eloquently, both with mathematical expressions and intuitive thought. You will be expected to link mathematics with the world around you – and in doing so will enable you to converse with a wide range of chemists, solving current real-world problems.

Grading

15% - Midterm and Final (7.5% each)

45% - Take home exams (15% each)

35% - Weekly Problem Sets

5% - Attendance and participation

Class Policies

- Due to the in-depth and comprehensive mathematical nature of this course, and the time required to undertake many physical chemistry problems, a large portion of exam work will be given in a take home format. These assignments are intended to be entirely performed on your own. Any evidence of group work,

collaboration, collusion, cheating, corroboration, or any other related offense will be fully investigated according to the rules set by the UVM Academic Integrity Office, and will simultaneously merit a zero for that assignment.

- The midterm and final will be primarily conceptual in nature. No calculators will be allowed.
- It is entirely acceptable and somewhat encouraged to work with your peers on the weekly problem sets. The problem sets will be assigned on Mondays and are due the following Monday – late assignments will not be accepted.

COVID-19 Policy: This class is intended to be fully in-person. Absences will only be excused with a valid medical exemption from a physician or other authorized source. Lectures will not be recorded by default, so requests for accommodations **must be made in advance of the class you will miss.**

Student Learning Accommodations

In keeping with University policy, any student with a documented disability interested in utilizing accommodations should contact SAS, the office of Disability Services on campus. SAS works with students and faculty in an interactive process to explore reasonable and appropriate accommodations, which are communicated to faculty in an accommodation letter. All students are strongly encouraged to meet with their faculty to discuss the accommodations they plan to use in each course. A student's accommodation letter lists those accommodations that will not be implemented until the student meets with their faculty to create a plan.

Contact SAS:

A170 Living/Learning Center;

802-656-7753;

access@uvm.edu

www.uvm.edu/access

Religious Holidays

Students have the right to practice the religion of their choice. If you need to miss class to observe a religious holiday, please submit the dates of your absence to me in writing by the end of the second full week of classes. You will be permitted to make up work within a mutually agreed-upon time.
<https://www.uvm.edu/registrar/religious-holidays>

Academic Integrity

The policy addresses plagiarism, fabrication, collusion, and cheating.
<https://www.uvm.edu/policies/student/acadintegrity.pdf>

Tentative Course Schedule (*subject to change*)

Week Number	Class Numbers	Topics	Reading
1	1-3	Introduction to QM, de Broglie, Bohr, uncertainty, classical waves, wavefunctions, operators, probability	Chs. 1-2
2	4-5	Particle in a box, correspondence principle, postulates of QM.	Chs. 3-4
3	6-8	Harmonic Oscillator, Hermite polynomials, Morse potential and anharmonicity, particle on a ring, angular momentum, spherical harmonics	Chs. 5-6
4	9-11	Spectroscopy, hydrogen atom	Chs. 13 & 6
5	12-14	Hydrogen atom, orbitals, variational method, multi-electron atoms, perturbation theory	Chs. 6-8
6	15-17	Pauli exclusion, Slater determinant, Hartree-Fock, MO theory, self-consistent field	Chs. 8-9
7	18-20	Diatomics, LCAO and hybrid orbitals, Huckel theory.	Chs. 9-11
8	21-22	Midterm. Computational chemistry.	
9	22-25	Introduction to statistical mechanics, first and second laws of thermodynamics, state functions, Boltzmann statistics, molecular energy levels.	Chs. 17-21
10	26-28	Partition functions and their evaluation	Chs. 17-21
11	29-31	Partition functions and thermodynamic parameters, internal energy, heat capacity, equipartition theorem.	Chs. 17-21
12	32-34	Equilibrium and chemical potential.	Ch. 26
13	35-37	Boltzmann distributions, kinetic theory of gases. Kinetics and rate laws.	Ch. 27
14	38-40	Kinetics, rate constants, transition state theory, Arrhenius equation. Review.	Chs. 28-29