Physical Chemistry for Graduate Students

CHE 457/505
Monday, Wednesday, and Friday
9:00-9:50 AM, Clemens Hall 06

Instructor: Prof. Alexey Akimov, NSC 716, 716-645-4140
alexeyak@buffalo.edu; http://www.chemistry.buffalo.edu/people/faculty/akimov/
Office Hours: Monday 4-5, Tuesday 4-5, and by appointment.
(No unannounced visits)

Course Website: https://ublearns.buffalo.edu

Homework: Homework must be turned in by the end of class on the due date (usually Monday). One day late: Earned score reduced by 50%. Two or more days late: No credit given. Exceptions will only be made in the case of documented emergencies.

Academic Integrity: Students should read the official UB Academic Integrity Policy found at: http://undergrad-catalog.buffalo.edu/policies/course/integrity.shtml

Grading Policy: ¼ Intro, ¼ Thermo/Statistical Mechanics, ¼ Quantum Chemistry, ¼ Course project. A letter grade will be assigned at the end of the course, based on the final percentage score. The cut off percentages used in the previous five years is as follows: 85 = A, 80 = A-, 75 = B+, 70 = B, 65 = B-, 60 = C+, 55 = C, 50 = C-, 45 = D, 40 = F. The instructor reserves the right to modify the grading scheme if this year’s class performs very differently from previous classes. The students should read the official UB Incomplete Policy found at: http://undergrad-catalog.buffalo.edu/policies/grading/explanation.shtml#incomplete

Students with Special Needs: Please inform the instructor of any special needs and
register with the Office of Accessibility Services (ODS) as soon as possible. See http://www.student-affairs.buffalo.edu/ods for details.

Student Resources: A. Ben Wagner, Chemistry Librarian, Science & Engineering Information Center, 118 Lockwood Library. Phone: (716) 645-1333. Email: abwagner@buffalo.edu. Info: http://library.buffalo.edu/bwagner

University Holidays (No Class): Labor Day (September 7) Fall Recess (November 25 and 27)

Total – 15 weeks

Tentative Schedule

Part I (Into)

Week 1: Mathematical background: matrix algebra, linear transformations, differential equations, integration, probability.
Week 2: Numerical methods and basics of programming
Week 3: Classical mechanics: equations of motion, Lagrangian & Hamiltonian dynamics

Part II (Quantum Chemistry)

Week 4: Introduction to QM: postulates of QM, bosons and fermions, spin.
Week 5: Particle in a box, harmonic oscillator, hydrogen atom
Week 6: Perturbation theory, variational method and Hartree-Fock theory
Week 7: Approximate and post-HF methods of quantum chemistry.
Week 8: Time-dependent Schrodinger equation: time-dependent perturbation theory, nonadiabatic dynamics, spectroscopy
Week 9: Intro in the group theory, quantum mechanics in condensed matter. Exam

Part III (Thermo/Statistical Mechanics)

Week 10: Phenomenological thermodynamics: variables, 3 laws of thermodynamics, equations of state
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Week 11: Statistical thermodynamics: ensembles, partition functions

Week 12: Computational approaches to thermodynamics and statistical mechanics: basics of molecular dynamics

Week 13: Phenomenological chemical kinetics: elementary reactions, order of reactions, enzymatic catalysis. Fall Recess

Week 14: Phenomenological chemical kinetics (continued)

Week 15: Statistical approaches to chemical kinetics: transition state theory, computational approaches

Part IV (Course project)

Week 16: Course project defense & Exam

The project is the pinnacle of the course. It will demonstrate your ability to apply the learned knowledge to real-world problems. It will be interspersed over the duration of the whole course. I encourage you to start it as early as you can, because it is expected to demonstrate a substantial involvement, creativity, and knowledge. Do not wait until the topic you want to focus on is covered in lectures.

The course project can be chosen by the student or can be assigned by the instructor (feel free to discuss it with me, when in doubts). The project must be well-documented and presented in front of the class. It may be of applied (computational, data analysis) or theoretical (theory analysis, derivations) origin. It may involve utilization of the third-party programs for performing computations, or it may be based on your own code/derivations.

The project will be graded as follows: 1/2 for the written presentation & content, 1/4 for the oral presentation, 1/4 for the review you will write on the assigned work or works of your colleagues.

Literature

There is no single textbook for the course. Here I only list a suggested reading for the course. I intentionally omit date/edition and publisher for it doesn’t really matter which one you will be using.

The textbooks I may be using:

1. Daan Frenkel, Berend Smit “Understanding Molecular Simulations: From Algorithms to Applications”;
2. M. P. Allen, D. J. Tildesley “Computer Simulation of Liquids”;
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3. Alan Hinchliff “Modelling Molecular Structures”;
4. Frank Jensen “Introduction to Computational Chemistry”;
5. “The Feynman Lectures on Physics”;
7. Robin M. Hochstrasser “Molecular aspects of symmetry”;
8. L. D. Landau, E. M. Lifshitz “Quantum Mechanics”;
9. I. Prigogine, “Introduction to Thermodynamics of Irreversible Processes”;
11. Tom M. Apostol “Calculus”: volume 1 - “One-Variable Calculus, with an Introduction to Linear Algebra”, volume 2 - “Multi Variable Calculus and Linear Algebra, with Applications to Differential Equations and Probability”
12. Furio Ercolessi “A molecular dynamics primer”;
15. R. McWeeny, B. T. Sutcliffe “Fundamentals of Self-Consistent-Field (SCF), Hartree-Fock (HF), Multi-Configuration (MC) SCF and Configuration Interaction Schemes”

The textbooks which were used in the past by other faculty:

1. Thermodynamics, Engel
2. Quantum Chemistry & Spectroscopy, Engel
3. Physical Chemistry: Berry, Rice & Ross
4. Physical Chemistry: Atkins/DePaula
5. Molecular Thermodynamics: R. E. Dickerson
6. Statistiscal Thermodynamics: D. A. McQuarrie

In case you can read Russian:

1. А. А. Соколов, И. М. Тернов, В. Ч. Жуковский “Квантовая Механика”
2. П. В. Елютин, В. Д. Кривченков “Квантовая Механика”
3. В. И. Минкин, Б. Я. Симкин, Р. М. Миняев “Теория Строения Молекул”