CHE 334: Physical Chemistry for Chemical Engineers LEC

Syllabus Revision 10. Last updated: August 31, 2021

Time and Location: MoWeFr 11:30 – 12:20, NSC 205, North Campus
The mode of instruction is *In person*

IMPORTANT: CHE 334 is a 2-credit course. CHE 334 will be a 10-week 3-hrs-per-week lecture course. Weeks 1 to 6 cover basic quantum theory, spectroscopy, molecular orbital theory. Weeks 7 to 10 cover band structure theory, quantum statistics, and selected other topics.

Instructor: Prof. Jochen Autschbach
Instructor email: jochena@buffalo.edu, Phone (for emergencies only): 716 430-4843
Instructor's Office Hours: Wed. 3:00 – 3:50 pm, NSC 732
Faculty mailboxes are located inside the Chemistry Department's main office, NSC 359

Grading Assistant (GA):
Herbert Ludowieg, NSC 738, herbertl@buffalo.edu
GA mailboxes are located in the hallway outside of 359 NSC

Important dates
Semester begins on Mon, Aug 30 (no class on Aug 30, Sep 1)
First class & Course Intro: Fri, Sep 3
Regular Lectures begin: Wed, Sep 8
Exam # 1: Mon, Oct 18 (date may change, check announcements at UBLearns)
Last Lecture: Fri, Nov 12
Exam # 2: Mon, Nov 15

Course web site: UBLearns, https://ublearns.buffalo.edu. The course web site contains downloadable (PDF) versions of the syllabus, homework, course notes, and announcements regarding the course. The instructor uses UBLearns to contact students by email. Make sure that your email address in UB's computer systems is up to date, and check your email frequently, esp. before exams and homework due days.

Learning Outcomes

Goal	Assessment
Be able to transfer knowledge	Solve problems in homework assignments, transfer knowledge to related but different problems during exams and practice exams
Knowledge of basic quantum theory, band structure concepts, quantum statistics	Homework and exam scores
Develop mathematical skills to be able to solve quantum mechanics problems	Homework scores
Be able to analyze band structures	Homework # 2, Exam #2

Textbook:

Recommended: *Quantum Theory for Chemical Applications* (QTCA) by J. Autschbach, Oxford University Press (2021). ISBN: 9780190920807. A textbook order has been placed with the UB North Campus book store, and the book can be ordered on-line here https://oxford.ly/3lVTUAh. You also have unlimited ebook access via your UB library account, so you don't need to look for pirated electronic versions. Go to https://library.buffalo.edu, search for the book's title, follow the Available Online link, and select the OSO version. You'll likely find QTCA useful. Among other resources, the book contains many worked-out exercises.

See the *Library Guide* posted on UBLearns for additional reading suggestions.

Course Content:

- Mathematical tools needed for the course. Functions, vectors, matrices. Dirac notation.
- Postulates of quantum mechanics. Atomic units.
- Particle-in-a-Box (PiaB).
- Basis set approximations and molecular orbitals.
- Hückel molecular orbital theory.
- Basic concepts of band structure theory: Bands, density of states, reciprocal lattice.
- Quantum Statistics vs. Boltzmann distribution.
- Misc. Topics (time permitting)

Exams, Assignments, Grades, Policies

The course's grade will be based on two graded homework assignments, and two exams. Grade details: Two homework sets, 20% of total grade each (40% combined). Two exams, 30% of total grade each (60% combined). The maximum total is 100%. The actual total percentage score for each student will be rounded to the nearest highest integer and then converted into letter grades as follows (the ranges are inclusive): 0 – 45 = F, 46 – 50 = D, 51 – 55 = D+, 56 – 60 = C-, 61 – 65 = C, 66 – 70 = C+, 71 – 75 = B-, 76 – 80 = B, 81 – 85 = B+, 86 – 90 = A-, 91 – 100 = A.

There is no 'extra credit' available; no exceptions. Regarding incomplete grades, see https://catalog.buffalo.edu/policies/grading.html

Homework and exam problems typically involve calculations and derivations to help familiarizing you with the (sometimes strange) properties of quantum systems. Exam questions may also be conceptual, such as: 'Explain what an orbital is', 'What is the origin of a spectroscopic selection rule?', etc. The answer then consists of a mix of text and relevant equations or sketches of functions.

You are welcome to use a Computer Algebra System (CAS) such as Wolfram Alpha, Mathematica, Maple, or Matlab, for your homework, as long as you include printouts of the CAS sessions to show your work. Also, variable names need to be explained to the grader, the steps need to be annotated, if necessary, figures need to be labeled properly, etc. Basically, put yourself in the grader's shoes and try to anticipate what he needs to have explained. The grader is not required to decipher incomprehensible CAS code or to guess what a plot is showing. Figuring out how

to get reliable answers from a CAS is potentially a better learning outcome than calculating standard integrals or derivatives yourself (as long as you know do it, in principle, without a CAS). The instructor often uses Mathematica for calculating the answers to homework problems for a course. UB has a campus license for several CASs. You can access those, and other software, via UB's Virtual Computing Lab. Instructions:
https://www.buffalo.edu/ubit/service-guides/software/my-virtual-computing-lab.html

Completed homework is due by the end of the lecture on the due-date listed on the assignment (usually one week after the homework was handed out). Late homework: 25% deduction off the total score per periods of 48 hrs late, starting at the end of class on the due-day. Homework assignments will be announced in class and posted on UBLearns. If you miss the class and are therefore unaware of posted homework, this is not an excuse for missing the due date. Attend all lectures.

Homework extensions without penalty, and requests for make-up tests, require *documentation* of a family or medical emergency or a similarly acceptable excuse.

Students must be familiar with and abide by the university's policies and procedures on Academic Integrity, available at the following link: Academic Integrity: https://catalog.buffalo.edu/policies/integrity.html

If you require reasonable accommodations to enable you to participate in this course, please contact the Office of Accessibility Resources in 60 Capen Hall, 716-645-2608 and also the instructor of this course during the first two weeks of class. The office will provide you with information and review appropriate arrangements for reasonable accommodations, which can be found on the web at:
http://www.buffalo.edu/studentlife/who-we-are/departments/accessibility.html

Technology Recommendations

To effectively participate in this course, regardless of mode of instruction, the University recommends you have access to a Windows or Mac computer with webcam and broadband. Your best opportunity for success in the blended UB course delivery environment (in-person, hybrid, and remote) will require these minimum capabilities listed on the following website:
https://www.buffalo.edu/ubit/service-guides/hardware/getting-started-with-hardware/purchasing-or-using-an-existing-computer.html