

CHE 320 LEC Physical Chemistry

Syllabus Revision 8. Last updated: February 1, 2021

Time and Location: TuTh 0800 – 0915.

The instruction mode for this course is Remote: real time and recorded. Three exams, weekly instructor office hours, and the first lecture on Feb. 2, will be during scheduled class time (see above, i.e. ‘real time’). All other lectures will be recorded. Homework will be taken on-line during multi-day time windows.

Instructor: Prof. Jochen Autschbach
Instructor email: jochena@buffalo.edu
Phone (emergencies only): 716 430-4843
Instructor’s Office Hours: Thu 0800 – 0915, via Zoom (see UBLearns for Zoom link)

Teaching Assistant (TA):

Farnoush Nourigheimasi, farnoush@buffalo.edu
TA will announce availability for Zoom meetings on UBLearns after classes start/

Important dates

Semester begins on Mon, Feb 1
Semester ends on Fri, May 7
First class & Course Intro: Tue, Feb 2
Exam # 1: Thu, Mar 11 (date may change, check announcements at UBLearns)
Exam # 2: Thu, Apr 8 (date may change, check announcements at UBLearns)
Exam # 3: Thu, May 6

Course web site: UBLearns, <https://ublearns.buffalo.edu>. The course web site contains downloadable (PDF) versions of the syllabus, homework, recorded lectures (video), 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 and announcements on UBLearns frequently, esp. before exams and homework due days.*

Learning Outcomes

Goal	Assessment (see ‘Course Grade’ for further details)
Be able to transfer knowledge	Solve problems in homework assignments, transfer knowledge to related but different problems in the exams
Knowledge of basic quantum theory and band structure theory	Homework and exam scores
Develop mathematical skills to be able to solve quantum mechanics problems	Homework scores
Knowledge of principles of important spectroscopic techniques (vibrational, rotational, & electronic excitations)	Homework and exam scores
Basic knowledge of computational chemistry	Homework and exam scores

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://global.oup.com/academic/product/quantum-theory-for-chemical-applications-9780190920807> and from other on-line book sellers. There is no required textbook, but you'll likely find QTCA useful. Among other resources, the book contains many worked-out exercises.

Optional: *Solids and Surfaces*, written by Roald Hoffmann, Wiley-VCH, 1988. This short book puts forward the orbital theory for crystals and crystal surfaces.

See the *Library Guide* for CHE 320 posted on UBLeads 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). Basic concepts of spectroscopy.

Many electron Hamiltonian, correlated electrons, Hartree product, orbitals.

Self-consistent field methods and electron orbitals.

Basis set approximations and molecular orbitals.

Hückel molecular orbital theory.

Basic concepts of band structure theory: Bands, density of states, reciprocal lattice.

Exams, Assignments, Grades, Policies

The course's grade will be based on three graded homework assignments, and three in-class exams. The lowest homework score will be discarded. Grade details: Two homework grades, 20% of total grade each (40% combined). Three exams, 20% 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 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.

Homework will be done on UBLeads approximately 1 to 2 weeks before each scheduled exam. Homework problem sets will be accessible for a time window of several days; details will be announced well before the homework is due. The exams will be taken on-line as well, during scheduled class time.

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 are able to provide printouts or screen shots of the CAS sessions upon request, to show your work. 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>

Homework extensions without penalty, and requests for make-up tests, require *documentation* of a family or medical emergency or a similarly acceptable excuse. If a student does not submit homework by the

end of the submission window, and there is no acceptable excuse, then there will be no points given for the homework. Likewise, failure to complete an exam within the scheduled time slot will result in the loss of points, possibly all of them, unless there is an 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 week 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>

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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>

The lectures recorded for this course use the H.264 video codec, and the sound codec is AAC. If your system's native browser has problems playing the videos with sound, please install the free VLC player on your system: <https://www.videolan.org/vlc/>