# Physical Chemistry Laboratory II
# Chemistry 330
## Monday, 1:00 PM - 5:50 PM, Baldy 8B
## Tuesday, 1:00 PM - 5:50 PM, Baldy 8B

Instructor: Dr. Jochen Autschbach
Office Hours: Wed 3 – 4 pm or by appointment
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Course Website: https://ublearns.buffalo.edu

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

Grading Policy: A letter grade will be assigned at the end of the course based on the final percentage score. The cut off percentages which will be employed are as follows: 90 = A, 83 = A-, 77 = 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, 118 Lockwood Library. Phone: 645-1333. Email: abwagner@buffalo.edu. Info: http://library.buffalo.edu/bwagner

**Computational Chemistry**

Computational modeling is becoming increasingly important in a variety of traditionally experimental disciplines. In chemistry, computations may be performed to predict new materials and their properties, gain a better understanding of the factors influencing chemical reactions, and aid characterization, to name a few important applications. Computations are no longer the domain of theoreticians, as increasing numbers of experimental research groups perform routine calculations to aid their work. This course will give the student an introduction to *practical* computational chemistry. An emphasis is placed on how to carry out a variety of different types of calculations and analyze the results. The theory underpinning the computational programs will be briefly outlined in pre-lab lectures, and can be further explored by the student in an independent project.

**Lab Reports**

It is expected that each report contains the following sections:

- Abstract
- Introduction
- Computational Details
- Results and Discussion – it is in this section that the students should answer all of the questions in the lab instructions
- Conclusion

Each student hand in their own lab reports. There will be no group work. During the first two weeks, the TA will further discuss requirements of a well-written lab report. Plagiarism includes copying material from reports of other students, from internet, or from published journal articles. Plagiarism will not be tolerated, and students will obtain a grade of 0% for lab reports which have been plagiarized in whole or in part. Each report must be written in your own words, and be based on your own computational results.

**Schedule**

The first and last day of classes are Monday January 30, and Friday May 12, respectively. Spring recess is from March 20 – 25. There will be four scheduled labs, with two consecutive classes devoted to each lab. On the first class day (listed in the schedule below), the instructor will introduce the lab, the TA will conduct pre-lab quizzes, and the remainder of the class time can be spent on performing the calculations. The TA will be available in the computer room during this time, and during the class of the following week, to help out in case there are questions or problems. Since WebMO can be accessed via the internet, work may be finished outside of the scheduled class time. Please don't expect the TA or the instructor to respond to help requests outside of the class and office hours. I.e. make the best use of the time when the TA is in the room with you and you can ask questions in person.

After completing the scheduled labs, each student is required to carry out a self-selected (independent) project. An outline of the proposed project must be approved by the lab instructor.

The students have four weeks to carry out the calculations for their proposed projects. An oral in-class presentation needs to be given about this work near the end of the semester.

The lab schedule is given below. The first date refers to the Monday and the second to the Tuesday section. The date listed is the day when the pre-lab quizzes will be conducted. The computer room will be open also a week following the listed date, as explained above.

1. Jan 30 / Jan 31: introduction and organization; demonstration of WebMO and Avogadro
2. Feb 6 / 7: **Lab 1 –** *"A Computational Experiment on the endo vs. exo Preference in a Diels-Alder Reaction"*
3. Feb 20 / 21: **Lab 2 –** *"Computational Studies of the Geometries and Properties of Carbon Single-Walled Nanotubes"*
4. Mar 6 / 7: **Lab 3 –** *"Computational Modeling of a Molecular Switch"*
5. Mar 27 / 28: **Lab 4 –** *"Computational Modeling of the Optical Rotation of Amino Acids"*
6. April 10/11: lab work for independent projects starts
7. May 8 / 9: 15-minute oral presentations of independent projects

**Grading Scheme, Late Work, and Due Dates**

There will be a pre-lab quiz before each of the four labs. Each quiz will contribute towards 2.5% of the total grade, for a total of 10%. Each of the four lab reports will be worth 15%, for a total of 60%. The independent project will be worth 30% of the grade, with 5% being given for an abstract outlining the proposed work, 10% for the oral presentation and 15% for the written report. *Unless there is a well-documented reason (medical or family emergency), students will not be allowed to make-up a lab. No points will be given for missed experiments.* To ensure balanced grading, the evaluation of a lab will only begin after all of the labs have been received from both sessions.

Reports are due in-class, at the beginning of class, at 1:00 pm, two weeks after the lab's start date listed above in the schedule. An exception is Lab no. 3, because of the Spring break. Please deliver your report for this lab to the TA or instructor before or on Mar 20 / 21. 20% will be deducted from work for every day that a report is late. The abstract of the proposed independent project *must* be approved by the TA and instructor before the project is carried out. The report is due on the same day when the presentation is given, but feel free to hand it in earlier. (That applies to all due dates, i.e. you may always submit reports before the last minute.) The student should consult the TA for any questions regarding regrades before approaching the instructor.

**Textbooks**

There are no required textbooks for the course. However, some additional reading is likely necessary. The following resources are recommended:

1. *Quantum Theory for Chemistry – Essential Elements*, by Jochen Autschbach (some printed copies available in the UB bookstore)

2. *Quantum Chemistry*, Fifth Edition or later, by Ira N. Levine
3. *Essentials of Computational Chemistry: Theories and Models*, by Christopher J. Cramer

**Learning Outcomes**

Upon completion of this course, students will be able to carry out the procedures and understand the concepts listed below. Unless otherwise stated, these learning outcomes will be assessed in each one of the four mandatory laboratory experiments, as well as in the independent project (as appropriate).

- Use the WebMO and AVOGADRO graphical user interfaces to build and pre-optimize molecular structures.
- Use modern quantum chemistry software, coupled with the WebMO interface, in order to carry out computations on molecules. The types of calculations which will be performed include: geometry optimizations, vibrational frequencies, transition state searches, molecular orbital calculation and visualization, calculations of molecular spectroscopic properties (ie. molar rotation, nuclear magnetic resonance chemical shifts). Most calculations will be carried out in the gas phase, however the effect of solvent will be considered in a few of the experiments.
- Understand the basic philosophies behind different computational methods including: molecular mechanics, as well as numerous quantum-chemical techniques (semi-empirical methods, density functional theory, *ab initio* methods including Hartree Fock theory and correlated wavefunction based techniques).
- Understand the difference between Slater type and Gaussian basis sets, as well as the nomenclature employed for Gaussian type basis functions. Be able to choose an appropriate basis set for a particular computational problem.
- Understand when to use explicit versus implicit solvation models, and when it is important to consider solvation effects in a calculation.
- Design and carry out a computational experiment (Assessment: Independent Project).
- Prepare a clear, concise, and visually appealing scientific presentation (using slide presentation software such as Power Point) and deliver it orally to a group of students and the instructors (Assessment: Independent Project).
- Scientific reasoning, scientific writing, scientific research, data analysis, analytical thinking as well as clear presentation of scientific results in graphic, written, and oral form.