Advanced Lab: Computation

Chemistry 370 - Tuesday 1:10-4pm

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Office hours M 9-10:30am, T 4-4:45pm, W 9-10am & by appointment

Course Description –

Like a traditional wet laboratory course, this course is designed to help promote your independence of thinking and hone your analytical skills; however this time we will be using the backdrop of computational chemistry. Although the words "computational chemistry" can be used to describe a plethora of methods used to help answer and refine questions from all the chemical sub-disciplines, within this milieu there are some important concepts that tend to be relatively universal and we will spend time discussing these issues and how to handle them in the laboratory setting. In particular, this course will highlight how computational methods can be integrated with kinetics to further the understanding of the mechanism of reaction systems and how computation can be used to gain knowledge about the structure and thermodynamics of single molecules. Finally, a small group project will allow you to pursue some of your own interests.

Attendance:

Attendance during the scheduled lab time is required.

Evaluation:

3 Reports (one after each unit)	45%
Homework (written and discussion format)	15%
Presentations (includes formal presentations of homework)	15 %
Quizzes	10 %
Final Project Paper	15 %

The total points earned and an evaluation of the student's participation in and preparedness for each laboratory workday will be used to assign an overall letter grade. It is expected that the student will have to do preparation and analysis outside of the listed class hours. Assignments in this course are often open-ended, so do your best work for the best results.

Laboratory Notebooks:

You are required to purchase and maintain a laboratory notebook. You may also find that a 3 ring binder will be handy to keep record of your computer programs and simulation results. Keeping an accurate and detailed lab notebook is critical as it is the only record of your work. While, there is no standard way to keep a lab notebook you will be expected to use it for the following items:

- General notes – assumptions, calculational ideas, data sources, etc. should be recorded here.
- Write with indelible ink
- After your simulation is completed, your notebook (in combination with printouts of your program) should provide enough information for others to reproduce your work and understand the theories lying behind the work.
- ***Notes for discussion. (An unconventional addition)*** Frequently we will read papers, etc. that require us to do homework/background investigation that may not directly relate to your laboratory project. The results of these investigations should also be written directly in your lab notebook or placed in the 3-ring binder.

Students with Disabilities

If you have a disability and therefore may have need of some type of accommodation(s) in order to fully participate in this class, please feel free to discuss your concerns in private with us and also to self-identify yourself to Erin Salva, Coordinator of Disability Services at PBX 5145 or via email at "salvae@ kenyon.edu". Please note that it is mandatory that you see Erin Salva for any accommodations to be given.

Students Athletes

Winter sport athletes must meet with me in the first week of classes to discuss any conflicts between the class assignments/requirements and the athletic requirements. ***Spring sport athletes*** must meet with me in the first week of practice to discuss any conflicts. This will allow us to find the best solution to any conflicts.

Academic Honesty

Please read Kenyon's statement "Academic Honesty and Plagiarism" found in the Course of Study. In short, materials submitted for grading must be your own work, that is, not a copy of someone else's work, even in part.

Changes

Any and all parts of this syllabus are subject to change. Notification of such changes will be made in class or via e-mail prior to taking effect.

Tentative Schedule

week		topic
1-5		~ REACTION SYSTEMS UNIT ~
1	sept 2	*Intro, Intro Kinetics & Berkeley Madonna*
2	sept 9	*Intro Modeling Methods/Philosophy, Methylene Blue Intro*
3	sept 16	*More Kinetics & Modeling Methylene Blue Kinetics*
4	sept 23	*More Kinetics & Modeling Methylene Blue Kinetics;*
5	sept 30 - **quiz**	*Reaction Systems Clean up, Project Determination*
6-9		~ SINGLE MOLECULE UNIT ~ (and project work on side)
6	oct 7	*Intro Gaussian & Methods*
7	oct 14	*More Gaussian w/ Azide Decomposition focus*
8	oct 21	*Gaussian & Azide Decomposition Clean up*
10-11		~ VISUALIZATION UNIT ~ (and project work on side)
9	oct 28- **quiz**	*Intro Molecular Visualization with PyMol*
10	nov 4	*More PyMol*
11-14		~ PROJECT WORK ~ *(and finish any lingering issues)*
FINAL		Final Project Paper due Dec 15 at 5pm

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Reports - Due Dates - TBA

A report will be written after each of the units, the reaction systems unit, single molecule unit and visualization unit.