Dr Gwen Shusterman: 350 SRTC, 503-725-3897, shustermang@pdx.edu

Office Hours: Tuesday 11-12, Wednesday 10-11 and after class meetings. Open door policy.


Learning Objectives:

1. Students can give/write down at least one reason we need quantum mechanics as a tool/theory to understand chemistry.
2. Students are able to apply the concept of boundary conditions to generate solutions to the Schrodinger Equation and determine quantum numbers.
3. Students can use the approximate Variational Method to calculate the energies and allowed states of a system.
4. Students can give a written description of the quantum origin of spectroscopy.
5. Students can deduce/determine structural information from spectroscopic data.
6. Students can effectively communicate scientific concepts to scientific and non-scientific audiences.
7. Students effectively and comfortably adopt various roles within the group structure, such as, manager, recorder or reporter.

Homework: Weekly problem assignments, unless otherwise announced, will be due on Wednesdays. Homework will be posted on the D2L page. Homework is due at class time. Late homework accepted through Friday for partial credit.

Simulations homework will also be posted on D2L. There will be worksheets posted and a very short quiz the day the assignment is due. Simulations will be assigned approximately once a week and be due on Mondays.

Computer software: The Mathcad program is available on the chemistry commons computers, SB 1 221. You can purchase a personal student copy through OIT for $20. This is a good tool for mathematically solving quantum problems, but not a requirement. I can set up a number of assignments that may be explored to further your understanding of key concepts, if requested. Only available for Windows.

For molecular modeling, Spartan software is available on the chemistry commons computers. This software is relatively expensive, but if you are interested in student version, you can look at the website: www.wavefun.com. There is also an iPad version, iSpartan that has a data bank of about 3000 molecules in it and costs $19.99.

Grades: Homework: 20%
In-Class participation: 15%
Midterm: 15%
Quizzes: 15%
Final: 35%

The midterm is tentatively scheduled for week 5, but this is subject to change.
In order to earn a C grade in this class you must satisfy the following:

1) Complete the homework problems and other out of class assignments earning 75% of possible points.
2) Fully participate during class activities, earning 85% of points possible (attendance and active participation)
3) Earn 80% on the simulation quizzes.
4) Show you can set up problems on exams, earning about 50% of points possible.

In order to earn an A grade in this class you must satisfy the following:

1) Complete the homework problems and other out of class assignments earning 85% of possible points.
2) Fully participate during class activities, earning 85% of points possible (attendance and active participation)
3) Earn 90% on the simulation quizzes.
4) Successfully complete problems on exam, earning about 80% of points possible.

The percentages given above may be adjusted downwards if the instructor feels performance on exams warrants this.

Success in this course will depend on your understanding of key concepts but also your ability to apply these concepts to solve problems. To earn an A or B grade you will need to develop strong math skills and will benefit from learning a symbolic math program such as MathCad. You must do homework assignments to succeed. Group work on homework is encouraged. I expect a significant portion of exam problems to be taken from the homework and our in class work.

What we will be doing; Scheduled lecture time will be used in several ways. Some class meetings will follow a standard lecture format. Other meetings will be used for problem solving sessions. This will include conceptual exercises, examples and problem solving practice. It is expected that you will attend class regularly and your participation during problem solving sessions is worth 15% of your grade.

You are responsible for any information or announcements given in class. Contact me as soon as possible if you miss any exams.

Disclaimer:

As the instructor of this course, I reserve the right to change the tentative schedule of topics, number and length of examinations, point distribution, course requirements, and percentages required for letter grades in order to better facilitate the learning process.
Below is a rough schedule of topics that we will cover. This document will continue to evolve, for updates, check D2L. With the new text, I’m not clear yet which sections of chapters we will use.

<table>
<thead>
<tr>
<th>Week</th>
<th>Chapter(s)</th>
<th>Topics</th>
</tr>
</thead>
</table>
| 1    | 7          | Why Quantum?  
          Classical Wave Equation  
          Math Review |
| 2    | 7,8        | Operators  
          Postulates  
          Particle in a Box |
| 3    | 8          | Particle in a Box  
          Schrodinger Equation – Eigen values  
          Tunneling |
| 4    | 8          | Harmonic Oscillator  
          Rigid Rotor – Microwave |
| 5    | 8          | Rigid Rotor  
          Midterm |
| 6    | 9          | H atom  
          Multi-electron Atoms  
          Angular Momentum |
| 7    | 10         | Huckel Theory |
| 8    | 10/12      | Molecular Orbital Theory |
| 9    | 12         | Molecular Spectroscopy |
| 10   | 13         | Electronic Spectroscopy  
          Review |

Policies:  
1. **Missing an Exam:** If you miss an exam, please contact me within 24 hours. I will allow you to reschedule your exam only if your absence was excused, EXCEPT in the following cases, where you will need to take the exam ahead of time:  
   a) Previously scheduled work or family commitments  
   b) School-sponsored field trips or athletic events  
   
   Illness, work conflicts and family emergencies are considered excused absences. Other instances will be evaluated on a case by case basis. All exams must be made up before the exams are passed back in class. In cases where it is not possible to schedule a makeup exam and your absence is excused, your final exam may be used to count for the missed midterm. Failure to notify me of the reason for your absence, as well as unacceptable excuses, will result in a score of zero for that exam.  

2. **Professional Demeanor:** It is expected that you will act with professional demeanor and attitude at all times. This includes, but is not limited to, being respectful at all times to the instructor and to your colleagues. **It also expected that you refrain excessive talking, cell phone use, or disruptive internet use in class.**  

3. **Dishonesty:** I trust that the work you do in this course is your own. Academic dishonesty will not be tolerated in this course. Cheating during any exam will be reported and the student will receive an “F” for the exam.  

4. **Accommodation:** If you have a physical or learning disability and you need extra accommodation, please be certain you are registered with Disability Services and make appropriate arrangements with me at the beginning of the term.