Physical Chemistry II CHEM 4424  
Physical & Environmental Sciences  
Spring 2015

A. COURSE INFORMATION  
Course number/section: CHEM 4424.001 and CHEM 4424.101  
Class meeting time: MWF 12:00 – 12:50 p.m.  
Class location: CI 106  
Course Website: https://bb9.tamucc.edu/

B. INSTRUCTOR INFORMATION  
Instructor: Timothy P. Causgrove  
Office location: CS 207  
Office hours: TBD  
Telephone: 825-2399  
e-mail: tim.causgrove@tamucc.edu  
Appointments: Additional appointments available by e-mail request

C. COURSE DESCRIPTION  
Catalog Course Description  
A continuation of CHEM 4423, including the study of chemical kinetics, electrochemistry, molecular structure, and quantum mechanics. Prerequisite: CHEM 4423. Safety training given during a laboratory meeting early in the semester is required for continued participation in this course.

Extended Course Description  
This course is the second semester of the two-semester physical chemistry sequence. It combines a lecture portion and a laboratory portion. The lecture portion of the course consists primarily of introductory quantum mechanics and its relation to spectroscopic observations. The course will also include reaction kinetics and kinetic mechanisms. The laboratory portion of the course will contain a mixture of traditional laboratory experiments, dry lab experiments and computer exercises.

D. PREREQUISITES AND COREQUISITES  
Prerequisites  
CHEM 4423  
Corequisites  
CHEM 4085

E. REQUIRED TEXTBOOK(S), READINGS AND SUPPLIES  
Required Textbook(s)
Elements of Physical Chemistry, 6th ed. by Atkins & DePaula (MacMillan Higher Education)

Optional Textbook(s) or Other References
None

Supplies
Scientific calculator, lab coat, goggles

F. STUDENT LEARNING OUTCOMES AND ASSESSMENT

Assessment is a process used by instructors to help improve learning. Assessment is essential for effective learning because it provides feedback to both students and instructors. A critical step in this process is making clear the course’s student learning outcomes that describe what students are expected to learn to be successful in the course. The student learning outcomes for this course are listed below. By collecting data and sharing it with students on how well they are accomplishing these learning outcomes students can more efficiently and effectively focus their learning efforts. This information can also help instructors identify challenging areas for students and adjust their teaching approach to facilitate learning.

By the end of this course, students should be able to:
1. Identify the solutions to the Schödinger equation
2. Extract physical quantities from wavefunctions
3. Calculate the allowed energy levels for molecules and atoms
4. Do calculations involving chemical kinetic equations

G. INSTRUCTIONAL METHODS AND ACTIVITIES

The laboratory grade will be based on laboratory assignments submitted for each experiment. It is expected that there will be nine laboratory assignments, with each weighted equally. Each laboratory assignment, which will vary depending on the lab activity, will be graded based on a maximum of 20 points. Laboratory experiments will be done in groups of two, and group may turn in one common assignment, or the students may turn in materials independently. Laboratory reports are generally due one week after the experiment. For non-laboratory (mostly computer) assignments, the work will be turned in individually and will generally be due during the lab period. Make-up lab attendance is intended only for those absent during a regular lab session.

H. MAJOR COURSE REQUIREMENTS AND GRADING

Your grade in this course will be based on both lecture and laboratory, broken down as follows:

<table>
<thead>
<tr>
<th>ACTIVITY</th>
<th>% of FINAL GRADE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exams (3)</td>
<td>45</td>
</tr>
</tbody>
</table>
## Quizzes

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Lab Average</td>
<td>25</td>
</tr>
<tr>
<td>Final Exam</td>
<td>20</td>
</tr>
</tbody>
</table>

Overall grades for the course (four hours credit) will be assigned according to a ten-point scale: A for >90%, B for 80-89%, C for 70-79%, D for 60-69%, and F for <60%. Rounding is at the discretion of the instructor.

### I. COURSE CONTENT/SCHEDULE

#### Lecture Schedule:

<table>
<thead>
<tr>
<th>DATE</th>
<th>TOPIC</th>
<th>CHAPTER</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/21</td>
<td>Introduction to Physical Chemistry II</td>
<td>-</td>
</tr>
<tr>
<td>1/23</td>
<td>Failure of classical mechanics</td>
<td>12.1-12.3</td>
</tr>
<tr>
<td>1/26</td>
<td>Schrödinger equation</td>
<td>12.4-12.5</td>
</tr>
<tr>
<td>1/28</td>
<td>The uncertainty principle</td>
<td>12.6</td>
</tr>
<tr>
<td>1/30</td>
<td>Translation – particle in a box</td>
<td>12.7</td>
</tr>
<tr>
<td>2/2</td>
<td>Rotation – particle on a sphere</td>
<td>12.8</td>
</tr>
<tr>
<td>2/4</td>
<td>Vibration – harmonic oscillator</td>
<td>12.9</td>
</tr>
<tr>
<td>2/6</td>
<td>Rydberg equation and hydrogenic atoms</td>
<td>13.1-13.2</td>
</tr>
<tr>
<td>2/9</td>
<td>Quantum numbers</td>
<td>13.3</td>
</tr>
<tr>
<td>2/11</td>
<td>Wavefunctions of the hydrogen atom</td>
<td>13.4</td>
</tr>
<tr>
<td>2/13</td>
<td>Atomic orbitals</td>
<td>13.5</td>
</tr>
<tr>
<td>2/16</td>
<td>Review for Exam #1</td>
<td>-</td>
</tr>
<tr>
<td>2/18</td>
<td>Electron spin</td>
<td>13.6</td>
</tr>
<tr>
<td>2/20</td>
<td>Selection rules and conservation</td>
<td>13.7</td>
</tr>
<tr>
<td>2/23</td>
<td>Orbital approximation and Pauli principle</td>
<td>13.8-13.9</td>
</tr>
<tr>
<td>2/25</td>
<td>Shielding and effective nuclear charge</td>
<td>13.10</td>
</tr>
<tr>
<td>2/27</td>
<td>Aufbau principle and spin correlation</td>
<td>13.11</td>
</tr>
<tr>
<td>3/2</td>
<td>Self-consistent field orbitals</td>
<td>13.14</td>
</tr>
<tr>
<td>3/4</td>
<td>Periodic trends</td>
<td>13.15-13.16</td>
</tr>
<tr>
<td>3/6</td>
<td>Spin-orbit coupling and term symbols</td>
<td>13.17</td>
</tr>
<tr>
<td>3/9</td>
<td>Valence bond theory</td>
<td>14.1-14.2</td>
</tr>
<tr>
<td>3/11</td>
<td>Diatomics and polyatomics</td>
<td>14.3-14.4</td>
</tr>
<tr>
<td>DATE</td>
<td>EXPERIMENT</td>
<td>SECTION</td>
</tr>
<tr>
<td>--------</td>
<td>-----------------------------------------------------</td>
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<tr>
<td>3/13</td>
<td>Hybrid orbitals</td>
<td>14.5</td>
</tr>
<tr>
<td>3/23</td>
<td><strong>Review for Exam #2</strong></td>
<td></td>
</tr>
<tr>
<td>3/25</td>
<td>LCAO-MO</td>
<td>14.8-14.9</td>
</tr>
<tr>
<td>3/27</td>
<td>MO diagrams – homonuclear diatomics</td>
<td>14.10</td>
</tr>
<tr>
<td>3/30</td>
<td>MO diagrams – heteronuclear diatomics</td>
<td>14.11</td>
</tr>
<tr>
<td>4/1</td>
<td>Polyatomics and the Hückel method</td>
<td>14.12-14.13</td>
</tr>
<tr>
<td>4/3</td>
<td>Computational chemistry</td>
<td>14.14-14.16</td>
</tr>
<tr>
<td>4/6</td>
<td>Rotational spectroscopy</td>
<td>19</td>
</tr>
<tr>
<td>4/8</td>
<td>Vibrational spectroscopy</td>
<td>19</td>
</tr>
<tr>
<td>4/10</td>
<td>Reaction rates and rate laws</td>
<td>19</td>
</tr>
<tr>
<td>4/13</td>
<td>Rate laws</td>
<td>10.3-10.5</td>
</tr>
<tr>
<td>4/15</td>
<td>Temperature dependence of rates</td>
<td>10.6-10.7</td>
</tr>
<tr>
<td>4/17</td>
<td>Collision theory and transition state theory</td>
<td>10.10-10.11</td>
</tr>
<tr>
<td>4/20</td>
<td>Specific rate expressions</td>
<td>11.1-11.3</td>
</tr>
<tr>
<td>4/22</td>
<td>Molecularity and multi-step reactions</td>
<td>11.4-11.5</td>
</tr>
<tr>
<td>4/24</td>
<td>Steady-state approximations</td>
<td>11.6-11.7</td>
</tr>
<tr>
<td>4/27</td>
<td><strong>Review for Exam #3</strong></td>
<td></td>
</tr>
<tr>
<td>4/29</td>
<td>Activation control and diffusion control</td>
<td>11.10-11.11</td>
</tr>
<tr>
<td>5/1</td>
<td>Temperature-derivative spectroscopy</td>
<td>-</td>
</tr>
<tr>
<td>5/4</td>
<td>Nuclear energy levels</td>
<td>21</td>
</tr>
<tr>
<td></td>
<td>Final Exam</td>
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</tr>
</tbody>
</table>

Note: Changes in this course schedule may be necessary and will be announced to the class by the Instructor. The assignments and exams shown are directly related to the Student Learning Outcomes described in Section F.

**Laboratory Schedule:**

<table>
<thead>
<tr>
<th>DATE</th>
<th>EXPERIMENT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/26</td>
<td>Math Review</td>
</tr>
<tr>
<td>2/2</td>
<td>Numerical Solution of the Schrödinger Equation</td>
</tr>
<tr>
<td>2/9</td>
<td>The Boltzmann Distribution</td>
</tr>
<tr>
<td>2/16</td>
<td><strong>Exam #1</strong></td>
</tr>
<tr>
<td>3/2</td>
<td>The Interpretation of the Emission Spectrum of Lithium</td>
</tr>
<tr>
<td>3/9</td>
<td>Simple and Extended Hückel Molecular Orbitals</td>
</tr>
<tr>
<td>Date</td>
<td>Topic</td>
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<tr>
<td>----------</td>
<td>-------------------------------------------------</td>
</tr>
<tr>
<td>3/16</td>
<td>Spring Break</td>
</tr>
<tr>
<td>3/23</td>
<td>Exam #2</td>
</tr>
<tr>
<td>3/30</td>
<td>The Variation Principle Applied to Vibrations</td>
</tr>
<tr>
<td>4/6</td>
<td>Excited State Properties of 2-Naphthol</td>
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<tr>
<td>4/13</td>
<td>Kinetics of Reduction of Glutathione</td>
</tr>
<tr>
<td>4/20</td>
<td>Kinetics continued</td>
</tr>
<tr>
<td>4/27</td>
<td>Exam #3</td>
</tr>
<tr>
<td>5/4</td>
<td>Make-up Lab</td>
</tr>
</tbody>
</table>

J. **COURSE POLICIES**

**Late Work and Make-up Exams**

There will be no make-up quizzes. Only the top 8 quizzes will count towards your grade. Late laboratory assignments will be assessed a penalty of 2 points in the first week after the due date and 10 points thereafter.

**Cell Phone Use**

Before you enter the classroom, turn off your cell phone.

**Laptop Use**

Laptops, tablets, and cell phones are not permitted during exams. You may NOT use your cell phone as a calculator.

**Missed Exam**

Students with a university approved absence (athletics, university field trips, etc.) MUST contact the instructor well in advance of the scheduled absence to arrange for an early exam. A written excuse from the university department involved is required. A written excuse from the university department involved is required. Students who do not contact the instructor prior to missing an exam do not have the right to a make-up exam, but special situations will be taken into account. In those cases, exams taken after the regularly scheduled exam may be more difficult and may not include bonus points.

K. **COLLEGE AND UNIVERSITY POLICIES**

- **Academic Integrity (University)**
  It is expected that university students will demonstrate a high level of maturity, self-direction, and ability to manage their own affairs. Students are viewed as individuals who possess the qualities of worth, dignity, and the capacity for self-direction in personal behavior.
  See Full University Policy at [http://catalog.tamucc.edu/content.php?catoid=10&navoid=313#Academic_Integrity](http://catalog.tamucc.edu/content.php?catoid=10&navoid=313#Academic_Integrity)
Classroom/Professional Behavior

Deadline for Dropping a Course with a Grade of W (University)
The grade of W will be assigned to any student officially dropping a course by Friday, April 10, 2015. No student is eligible to receive a W without completing the official drop process by this deadline. Visit the Office of the University Registrar for the Course Drop Form that must be submitted. After April 10, 2015 a student will not be allowed to drop a course.

Grade Appeals (College of Science and Engineering)
As stated in University Procedure 13.02.99.C2.01, Student Grade Appeal Procedures, a student who believes that he or she has not been held to appropriate academic standards as outlined in the class syllabus, equitable evaluation procedures, or appropriate grading, may appeal the final grade given in the course. The burden of proof is upon the student to demonstrate the appropriateness of the appeal. A student with a complaint about a grade is encouraged to first discuss the matter with the instructor. For complete details, including the responsibilities of the parties involved in the process and the number of days allowed for completing the steps in the process, see University Procedure 13.02.99.C2.01, Student Grade Appeal Procedures. These documents are accessible through the University Rules website at http://www.tamucc.edu/provost/university_rules/index.html, and the College of Science and Engineering Grade Appeals webpage at http://sci.tamucc.edu/students/GradeAppeal.html. For assistance and/or guidance in the grade appeal process, students may contact the chair or director of the appropriate department or school, the Office of the College of Science and Engineering Dean, or the Office of the Provost.

Disability Services
Disability Services (DS) is the hub for coordinating services and accommodations to ensure accessibility and utilization of all programs for all Texas A&M University-Corpus Christi students with disabilities. Our services are designed to meet the unique educational needs of enrolled students with documented permanent or temporary disabilities. DS provides intake and consultation services to students seeking to register with our office. DS reviews an individual’s documentation of disability and assesses eligibility for services and the determination of reasonable accommodations. For more information visit the Disability Services Office at 116 Corpus Christi Hall or go to http://disabilityservices.tamucc.edu/

L. GENERAL DISCLAIMER
I reserve the right to modify the information, schedule, assignments, deadlines, and course policies in this syllabus if and when necessary. I will announce such changes in a timely manner during regularly scheduled lecture periods.