CHEM 501

California State University San Marcos • NEW COURSE • FORM C

ORIGINATOR'S SECTION:

1. College:

☐ **CHABSS** ☐ **CoBA**
☐ **CoEHHS** ☒ **CSM**

Desired Term and Year of Implementation (e.g., Fall 2008):

Fall 2017

2.Course is to be considered for G.E.? (If yes, also fill out appropriate GE form*) ☐ Yes ☒ No

3. Course will be a variable-topics (generic) course? ☐ Yes ☒ No
("generic" is a placeholder for topics)

4. Course abbreviation and Number:* CHEM 501

5. Title: ***(Titles using jargon, slang, copyrighted names, trade names, or any non-essential punctuation may not be used.)***
Computational Physical Chemistry

6. Abbreviated Title for PeopleSoft:
(no more than 25 characters, including spaces)
Comp Physical Chem

7. Number of Units: 4

8. Catalog Description: ***(Not to exceed 80 words; language should conform to catalog copy. Please consult the catalog for models of style and format; include all necessary information regarding consent for enrollment, pre- and/or corequisites, repeated enrollment, crosslisting, as detailed below. Such information does not count toward the 80-word limit.)***

Introduces students to computational methods as applied to some of the major theoretical ideas of Physical Chemistry. The concepts to be covered will include examples from: Classical Chemical Thermodynamics, Statistical Thermodynamics, Chemical Kinetics, Quantum Chemistry, and/or Molecular Modeling. The course is designed to build on previous knowledge of Physical Chemistry gained at the undergraduate level. *Prerequisite: A minimum grade of C (2.0) in CHEM 401 and CHEM 402 or classified graduate standing.*

9. Why is this course being proposed?

This course is being proposed as part of the new Masters in Chemistry program. CHEM 501 will serve as a required core course in the option in chemistry.

10. Mode of Instruction*
For definitions of the Course Classification Numbers:
http://www.csusm.edu/academic_programs/curriculumscheduling/catalogcurricula/DOCUMENTS/Curricular_Forms_Tab/Instructional%20Mode%20Conventions.pdf

Type of Instruction	Number of Credit Units	Instructional Mode (Course Classification Number)
Lecture	3	C-02
Activity	1	C-07
Lab		

11. Grading Method:*
☒ Normal (N) *(Allows Letter Grade +/-, and Credit/No Credit)*
☐ Normal Plus Report-in-Progress (NP) *(Allows Letter Grade +/-, Credit/No Credit, and Report-in-Progress)*
☐ Credit/No Credit Only (C)
☐ Credit/No Credit or Report-in-Progress Only (CP)

12. If the (NP) or (CP) grading system was selected, please explain the need for this grade option.

13. Course Requires Consent for Enrollment? ☐ Yes ☒ No

☐ Faculty ☐ Credential Analyst ☐ Dean ☐ Program/Department - Director/Chair

14. Course Can be Taken for Credit More than Once? ☐ Yes ☒ No
If yes, how many times? (including first offering)

15. Is Course Crosslisted: ☐ Yes ☒ No

If yes, indicate which course and check "yes" in item #22 below.

16. Prerequisite(s): ☒ Yes ☐ No CHEM 401 and CHEM 402 or classified graduate standing.

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* If Originator is uncertain of this entry, please consult with Program/Department Director/Chair.

17. Corequisite(s): ☐ Yes ☒ No

18. Documentation attached:
☐ Syllabus ☒ Detailed Course Outline

19. If this course has been offered as a topic, please enter topic abbreviation, number, and suffix:*

20. How often will this course be offered once established?* Once every year or every 3rd semester.

PROGRAM DIRECTOR/CHAIR - COLLEGE CURRICULUM COMMITTEE SECTION:
(Mandatory information – all items in this section must be completed.)

21. Does this course fulfill a requirement for any major (i.e., core course or elective for a major, majors in other departments, minors in other departments)? ☒ Yes ☐ No

If yes, please specify:
Core course in the Chemistry option of the Masters of Science in Chemistry, and an elective in the Biochemistry option.

22. Does this course impact other discipline(s)? ***(If there is any uncertainty as to whether a particular discipline is affected, check "yes" and obtain signature.)*** ☐ Yes ☐ No

If yes, obtain signature(s). Any objections should be stated in writing and attached to this form.

Discipline _____ Signature _____ Date _____ Support _____ Oppose

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SIGNATURES : (COLLEGE LEVEL) :

P. Jasien 8/4/2016
1. Originator (please print or type name) Date

8/9/16
2. Program Director/Chair Date

12/14/16
3. College Curriculum Committee Date

12/14/16
4. College Dean (or Designee) Date

(UNIVERSITY LEVEL)

5. UCC Committee Chair Date

6. Vice President for Academic Affairs (or Designee) Date

7. President (or Designee) Date

Office of Academic Programs PS Banner: _____ Catalog _____ Revised 3/28/2007

* If Originator is uncertain of this entry, please consult with Program/Department Director/Chair.

RP ____ Tracker ✓

Chemistry 501
Computational Physical Chemistry
MW 1500-1700
Fall 2015

Dr. Paul Jasien
Office: SCI2-333
Phone: 760-750-4135
email: jasien@csusm.edu

Introduction: This course presents an introduction to computational chemistry methods as applied to physical chemistry. The content of this course will include some background theory and applications of the various modeling techniques, as well as a number of hands-on activities using available software.

Course Description: Designed to introduce students to computational methods as applied to some of the major theoretical ideas of Physical Chemistry. The concepts to be covered will include examples from: Classical Chemical Thermodynamics, Statistical Thermodynamics, Chemical Kinetics, Quantum Chemistry, and/or Molecular Modeling. The course is designed to build on previous knowledge of Physical Chemistry gained at the undergraduate level.

Prerequisites: The prerequisites for this course are successful completion of one full year of Physical Chemistry (CHEM 401 and CHEM 402).

Text: There is no specific text for this course. Readings from the literature will be used to introduce certain concepts. Students will be required to consult the primary literature for examples of various research applications of the various computational methods that have been studied. In addition, the instructor will provide supplemental reading material as required.

Topics

1. $\Delta H°$ as a Function of Temperature
2. Determination of $\Delta H°$ Using the van't Hoff & Claussius-Clapeyron Equations
3. A Statistical View of S
4. Calculation of $\Delta G°$ and K as Functions of Temperature
5. Chemical Kinetics Using Differential Equations
6. Rate Processes Using Stochastic Simulations
7. Atomic Structure and Spectra
8. A Molecular Orbital Description of Bonding
9. Potential Energy Surfaces of Molecules
10. Spectroscopic Properties of Molecules
11. Potential Energy Surfaces for Non-covalent Interactions
12. Classical Models for Potential Energy Surfaces
13. A Theoretical Description of Chemical Reactions
14. Spectroscopic Properties of Molecules from Quantum Mechanics
15. Quantitative Structure Property Relationships (QSPR)

Student Learning Outcomes: During this course, students will:

1. Apply computational simulation methods to predict the behavior of chemical systems.
2. Investigate how chemical and physical parameters affect experimentally observable quantities as given by the fundamental equations of physical chemistry.
3. Examine statistical relationships between various chemical and physical properties of molecules.
4. Apply quantum mechanical methods in order to predict reaction energies, molecular structure, and spectroscopic properties.

Grading: The course grade will be determined by the student's performance on in-class exercises, short written reports, mini-projects, and the final exam.

Item	Points
In-class Lab Reports (13 x 10 pts)	195
Short Literature Reports (4 x 100 pts.)	400
Mini-Projects 240 (2 x 120 pts.)	
Final Exam	165
	1000

A- ≥ 900; B- ≥ 800; C- ≥ 700; D- ≥ 600 (absolute point scale)

The final exam is scheduled for: XX from YY-ZZ.

In-class Lab Reports
These reports will be due at the end of class and will be a summary of the computational work you have done in that day's class. Needless to say, you must attend class in order to complete these reports.

Short Literature Reports
These reports are based on a publication from the primary literature that you have chosen to read. After reading the paper you are required to write a two page (word-processed, 12-pt font, 1 inch margins) summary of the paper. The summary should include sections on: (i) the purpose of the work, (ii) the computational methodology used, (iii) the relevant data obtained, (iv) the conclusion, and (v) a critique of the computational methodology used to solve the problem. Appropriate publications will be chosen in consultation with the instructor, although it is the responsibility of the student to search the literature for the publications to be considered.

Mini-Projects
These will be short assignments in which you will be asked to solve a chemical problem using computational methods that have been presented in class. A short abstract (300 words or less) as is usually written for a formal publication is required. This abstract should concisely describe the purpose, methods, major results, and conclusion of your research. In addition, you will need to turn in publication quality tables concisely summarizing all of your calculations.

CSUSM Writing Requirement
The University writing requirement will be satisfied through the written lab reports for the in-class computational exercises, the literature reports, and the reports for the mini-projects.

Office Hours: My official office hours for the semester will be: XXX. I also encourage you make an appointment to see me at other times if you need help.