Spring 2019

CHEM 491-813: Independent Study

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NJIT New Jersey Institute of Technology

THE COLLEGE OF SCIENCE AND LIBERAL ARTS

THE DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE

Chem 491:
Spring 2019 Course Syllabus

NJIT Academic Integrity Code: All Students should be aware that the Department of Chemistry & Environmental Science (CES) takes the University Code on Academic Integrity at NJIT very seriously and enforces it strictly. This means that there must not be any forms of plagiarism, i.e., copying of homework, class projects, or lab assignments, or any form of cheating in quizzes and exams. Under the University Code on Academic Integrity, students are obligated to report any such activities to the Instructor.
Looking up course materials such as past exams or homework solutions on external websites constitutes as **cheating**.
Posting of course materials on external websites without the approval of the instructor violates intellectual property laws and hence **strictly forbidden**.

COURSE INFORMATION

Course Description: Chem 491, Independent Study.

This course will cover material taught in the Chem 336: Physical Chemistry III course, but in a reading course format instead of a traditional lecture format.

Course-Section and Instructors

Course-Section	Instructor
Chem 491-813	Dr. Krishtal

Office Hours: Monday 10:00am – 11:20am
Tuesday 02:30pm – 03:50pm
Thursday 01:00pm – 02:20pm
Friday 01:00pm – 02:20pm
In case of schedule conflicts, you can make an appointment outside of these hours by emailing krishtal@njit.edu.

Required Textbook:

Title	Physical Chemistry
Author	Peter Atkins and Julio de Paula
Edition	10^{th} or 11^{th}. For approval of older editions please contact the instructor
Publisher	Freeman for 10^{th} edition; Oxford for 11^{th} edition
ISBN #	10^{th} edition: 978-1-4292-9019-7; 11^{th} edition: 978-0-19-876986-6

University-wide Withdrawal Date: The last day to withdraw with a **W** is Monday, April 8, 2019. It will be strictly enforced.

Learning Outcomes:

At the end of 491, you will be able to

1. **Describe the concept of energy quantization and wave-particle duality of light and matter**
2. **Discuss differences and similarities between classical and quantum chemical models**
3. **Construct the Schrödinger equation for simple systems**
4. **Normalize a wave function and calculate the probability density of a system in a region**
5. **Construct quantum chemical operators and determine expectation values of observables**
6. **Describe the solution of the Schrödinger equation for a free motion in one dimension and confined motion in one and two dimensions, and calculate their properties.**
7. **Use the separation of variables technique**
8. **Describe the solution of the Schrödinger equation for a harmonic oscillator and calculate it's properties.**
9. **Describe the solution of the Schrödinger equation for a particle on a ring and particle on a sphere and calculate their properties.**
10. **Describe the solutions of the Schrödinger equation for hydrogenic atoms and their properties: quantum numbers, orbital energies, classification in shells**
11. **Construct a wave function for a many-electron atom using the orbital approximation**
12. **Interpret atomic spectra of hydrogenic atoms and complex atoms using selection rules and assign term symbols to electronic states of atoms**
13. **Explain the concept of hybridization and molecular orbital theory**
14. **Assign ground state electron configurations to homo- and heteronuclear diatomic molecules**
15. **Use the variation principle to calculate energies of heteronuclear diatomic molecules**
16. **Use the Hückel approximation to calculate the -electron binding energy in aromatic molecules.**
17. **Explain the fundamental concepts of absorption and emission spectra**
18. **Calculate moments of inertia of simple molecules and classify them as rotors**
19. **Interpret microwave and Raman rotation spectra of molecules using selection rules**
20. **Interpret IR-spectra of diatomic and polyatomic molecules using selection rules**
21. **Assign term symbols to electronic states of diatomic molecules**
22. **Interpret electronic spectra of molecules using selection rule**
23. **Explain the fluorescence and phosphorescence decay mechanisms**

POLICIES

All CES students must familiarize themselves with, and adhere to, all official university-wide student policies. CES takes these policies very seriously and enforces them strictly.

Grading Policy: The final grade in this course will be determined as follows:

Weekly assignments	70%
Final project	30%

Your final letter grade in this course will be based on the following tentative curve:

A	90.0%-100%	**C**	70.0%-74.9%
B+	85.0%-89.9%	**D**	60.0%-69.9%
B	80.0%-84.9%	**F**	<60.0%
C+	75.0%-79.9%		

Attendance Policy: Weekly class meetings are mandatory.

Weekly assignments: Every week, an assignment will be given as a reading in the book and a project in the form of exercises, presentation, calculation or research from external sources. At each meeting, the assignment from previous week will be collected and graded. The

grading rubric for each assignment can differ depending on its nature and will be specified when assigned. Assignments can only be submitted during the weekly meetings, unless there is a valid reason approved by the Dean of Students. The average grade of all assignments will count for 70% of the course. No assignments will be dropped.

Final project: In the last month of the course, a final project will be assigned to each student which will replace the final exam. The final project grade will count to 30% of the final grade.

ADDITIONAL RESOURCES

Accommodation of Disabilities: Office of Accessibility Resources and Services (***formerly known as Disability Support Services***) offers long term and temporary accommodations for undergraduate, graduate and visiting students at NJIT.

If you are in need of accommodations due to a disability please contact Chantonette Lyles, Associate Director at the Office of Accessibility Resources and Services at 973-596-5417 or via email at lyles@njit.edu. The office is located in Fenster Hall Room 260. A Letter of Accommodation Eligibility from the Office of Accessibility Resources Services office authorizing your accommodations will be required.

For further information regarding self-identification, the submission of medical documentation and additional support services provided please visit the Accessibility Resources and Services (OARS) website at:

- http://www5.njit.edu/studentsuccess/disability-support -services/

Important Dates (See: Fall 2018 Academic Calendar, Registrar)

Date	Day	Event
January 22, 2019	T	First Day of Classes
February 1, 2019	F	Last Day to Add/Drop Classes
March 17 - 24, 2019	Su - Su	Spring Recess
April 8, 2018	M	Last Day to Withdraw
April 19, 2018	F	Good Friday – University Closed
May 7	T	Last Day of Classes, Friday Classes Meet
May 8-9	W - R	Reading Days
May 10 - 18	F - R	Final Exam Period

Course Outline

Week	Chapter	Topic
1 R 1/24	7A	Quantum mechanics vs classical mechanics
2 R 1/31	7B	Wavefunctions: normalization, quantization, probability density
3 R 2/7	7C	Operators and observables
4 R 2/14	8A	Translational motion: Free motion and particle in a box
5 R 2/21	8B	Vibrational motion: Harmonic oscillator
6 R 2/28	8C	Rotational motion: Particle on a ring, particle on a sphere
7 R 3/7	9A	Hydrogenic atoms
8 R 3/14	9B	Many-electron atoms
9 R 3/21	9C	Atomic spectra
10 R 3/28	10A	Valence bond theory
11 R 4/4	10B, C, D	Molecular Orbital Theory
12 R 4/11	10E	Hückel approximation, computational chemistry
13 R 4/18	12B, C	Rotational spectroscopy
14 R 4/25	12D	Vibrational spectroscopy
15 R 5/2	13	Electronic spectra