1. Course Information

Course Code & Name: Chem493, Quantum Chemistry
Semester & Year: Spring 2017-2018
Time & Location: Wednesdays 14:40-18:30, K-15

2. Instructor Information

Name: M. Fatih Danışman
Office Address: O-318 Chemistry
Office Hours: No fixed office hours. Take appointment (through e-mail) before coming to my office
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3. Course Description

In this course sevreal mathematical and quantum mechanical comptutaion and data analysis softwares will be introduced. Concepts discussed in Mathematics (257) and Quantum Chemistry (350) courses, like Fourier analysis, linear algebra, numerical methods, aprroximate quantum chemistry methods, will be revisited and their applications on "complex" chemical systems will be demonstrated by using the above mentioned computer programs.

4. Course Materials & Resources

Textbooks:

Quantum Chemistry Lecture Notes by Prof. İlker Özkan (will be provided to you via ODTÜClass in pdf format).

Quantum chemistry Levine, Ira N., 1937- Upper Saddle River, N.J. : Prentice Hall, c2000.
Call no: QD462 .L48 2009 (6th edition) (will be referred to as **L**)

The chemistry maths book Steiner, E., Oxford ; New York : Oxford University Press, 2008.
Call no: QA37.2 .S7985 (2nd edition) (will be referred to as **S**)
Electronic version can be accessed at:
http://app.knovel.com/web/toc.v/cid:kpCMBE0004/viewerType:toc/root_slug:chemistry-maths-book

Physical chemistry Keith J. Laidler, John H. Meiser, Bryan C. Sanctuary. Laidler, Keith James, Boston: Houghton Mifflin, c2003. Call no: QD453.3 .L35 2003 (will be referred to as **LKJ**)

Physical chemistry Atkins, P. W., de Paula J., Oxford University Press, 2006.
Call no: QD453.2 .A88 2006 (8th edition) (will be referred to as **A**)
Online Resource Center: http://global.oup.com/uk/orc/chemistry/pchem10e/

Physical chemistry : a molecular approach McQuarrie, Donald A., Sausalito, Calif. : University Science Books, c1997. Call no: QD453.2 .M394 (will be referred to as **M**)

Molecular quantum mechanics Atkins, P. W., Oxford University Press, 2005.
Call no: QD462 .A85 2005, Online Resource Center: http://global.oup.com/uk/orc/chemistry/mqm5e/

Fundamentals of physics Halliday, D., Resnick R., Walker J.,John Wiley Sons Inc., 2008.
Call no: QC21.3 .H35 2005 (7th edition) (8th edition will be referred to as **H**)

WWW:

Qunatum Tutorials of Prof. Frank Rioux at St. John's University and College of St. Benedict may be very helpful and can be accessed at the foolowing address:
http://www.users.csbsju.edu/~frioux/workinprogress.html

Software:

Mathcad: This is a powerful and easy to use/learn math software. Since it is based on a visual input format that uses standard mathematical notation (rather than text input that many other math software, like *Mathematica*, use) it is very easy to learn how to use it.

Origin Pro: Origin is a scientific graphing and data analysis software.

Hyperchem: "HyperChem is a molecular modeling environment that is known for its quality, flexibility, and ease of use. Uniting 3D visualization and animation with quantum chemical calculations, molecular mechanics and dynamics, HyperChem puts molecular modeling tools at your fingertips. It includes all the components of structure, thermodynamics, spectra, and kinetics."

5. Contents

Section numbers corresponding to each topic, from the references given above, are indicated in parantheses, next to topic titles.

1. **Numerical methods, from S (Mathcad, Origin):**
   20.3 Solutions of ordinary equations
   20.4 Interpolation
   20.5 Numerical integration – differentiation
   20.6 Methods in linear algebra

2. **Signal processing and analysis, from S (Mathcad, Origin):**
   21.7 Continuous distributions
   21.8 Gaussian distribution and peak shapes
   21.10 Least squares fitting
   Convolution-deconvoluiton
   Smoothing

3. **Particle in a circular box, from S (Mathcad):**
   14.5 Particle in a circular box:
   > DMEigler's 1993, Science article will be treated and quantum mechanical concept of superposition of states and curve fitting proceudres will be demonstrated.

4. **The variation method, from L (Mathcad):**
   8.1 The variation theorem
   8.4 Simultaneous linear equations
   8.5 Linear variation functions
   8.6 Matrices, eigenvalues and eigenvectors

5. **Fourier transforms, from S (Mathcad, Origin):**
   15.6 Fourier transforms:
   > Applications of Fourier analysis in signal processing, diffraction and IR spectroscopy will be disccused

6. **Hartree-Fock Self-Consistent-Field Method, from L (Mathcad, Hyperchem):**
   11.1 The Hartree-Fock self-consistent-field method
   13.16 The Hartree-Fock method for molecules

7. **Semiempirical and Molecular-Mechanics Treatments of Molecules, from L (Mathcad, Hyperchem):**
   16.3 The Huckel MO method
   16.5 General semiempirical MO methods
   16.6 The Molecular-Mechanics method

6. Exams and Grading Policy

Your performance in this course will be assessed by two projects

Midterm project/manuscript	40%
Final project/manuscript	60%

7. University Policies

It is very important that you know and understand the university regulations regarding academic integrity, since you are expected to and should act according to these rules throughout your university life. Below I quote the abovementioned academic integrity code.

MIDDLE EAST TECHNICAL UNIVERSITY ACADEMIC INTEGRITY GUIDE FOR STUDENTS

Middle East Technical University aims to access knowledge and produce, apply and disseminate it for the social, cultural, economic, scientific and technological development of both our society and humanity by carrying out activities of education, research and community services at universal standards, and to educate individuals who are equipped with this knowledge and at the same time who respect knowledge and the rights of others. In accordance with this aim, all members and students of our university adopt the following METU Code of Honor:

> "*As reliable, responsible and honorable individuals, all members of Middle East Technical University embrace only the success and recognition they deserve, and act with integrity in the use, evaluation and presentation of facts, data and documents*."

What is academic integrity?

Academic Integrity entails carrying out original work and sharing ideas and findings of others provided that the source is cited.

What are infringements of academic integrity?
1. Plagiarism,
2. Cheating,
3. Presenting or submitting in different courses the whole or part of a personal study, homework or project done previously with a different purpose without citing the source,
4. Indicating sources that do not actually exist as references or creating a false data set,
5. Conducting academic work on behalf of other students,
6. Behaving in a manner so as to obtain an unfair advantage (obtaining false medical reports, declaring false excuses for period extensions and make-ups, transferring or obtaining the right of enrollment to a course in exchange for a personal gain, etc.),
7. Producing or making use of fraudulent documents (reference letters, medical reports, proficiency documents/scores, transcripts, etc.)
8. Impersonating someone else in an exam; having someone else impersonate oneself.

Plagiarism:

"Plagiarism is intentionally or unintentionally acquiring and using someone else's ideas and opinions and presenting them as if one's own without making a reference to or citing the source." (ODTÜ UEAM)

Detailed information on the types of plagiarism can be found at the address http://ueam.metu.edu.tr/intihal.

Cheating:

Cheating is described as any attempt or action involving the use of disallowed sources secretly while answering exam questions. Each item below is within the scope of cheating:

1. Peeking at another student's paper during an exam,
2. Peeking at another student's paper during an exam and copying the answers onto one's own paper,
3. Talking to other students during the exam,
4. Any kind of sharing of information and sources during an exam (exchanging notes, etc.)
5. Taking exam questions and/or answers out of the exam hall without permission by writing them down or photographing them,
6. Transmitting exam questions to someone else or obtaining answers through cellular phones or any other electronic gadget during the exam,
7. Writing notes concerning the content of the exam on desks and accessories used during the exam, or on one's body or elsewhere,
8. Having someone else do the academic work; doing work to be done individually with other students,

9. Submitting to the course instructor reports/documents such as homework or projects prepared by others as if one's own work.

Disciplinary action to be taken against cheating is arranged by the Rules and Regulations Governing Student Disciplinary Actions in Institutions of Higher Education, which can be found at the address http://oidb.metu.edu.tr/yonetmelikler.

Reminders for students:
1. Carefully read the documents concerning academic integrity which have been issued to you and the related regulations on the University's website.
2. Learn in detail which situations fall into the scope of plagiarism in academic studies from relevant resources (e.g. ODTÜ UEAM website). In cases of plagiarism, excuses such as "I wasn't aware that what I've done is within the scope of plagiarism" are unacceptable. Be informed that the responsibility for such behavior is entirely yours.
3. Use your own ideas in all of your work such a piece of homework, project etc. Indicate the source of any thought, idea, text, document or finding which does not belong to you.
4. Prepare all your homework, projects, reports etc. by referring to the accessible original (primary) sources.
5. During examinations, abide by the rules in the Middle East Technical University Guide for Rules To Be Followed in an Examination Environment as well as the rules determined by the instructor of the course.