Lecturer: Mehmet Fatih Danışman
Office: O-318
e-mail: danisman@metu.edu.tr
Class Meeting Times and Locations: Wednesday: 12:40-13:30; K-05Thursday: 10:40-12:30, K-07

1. Course Description

The objectives of this course is to give basic knowledge on molecular spectroscopy, statistical thermodynamics, and reaction dynmics.

2. Course Materials & Resources

Textbook:

Physical chemistry Atkins, P. W., de Paula J., Oxford University Press, 2006.
Call no: QD453.2 .A88 2006 (8th edition)

Refrence textbooks:

Chem 350 lecture notes prepared by Prof. İlker Özkan.

Thermodynamics, statistical thermodynamics, and kinetics, Engel, T. and Reid, P., Pearson, 2013. Call no: QC311.5.E65 2013

Statistical Mechanics: a concise introduction for chemists. Widom, B., Cambridge University Press, 2002. Call no: QC174.8 .W53 2002

Spectra of Atoms and Molecules Bernath, P. F., Oxford University Press, 1995. Call no: QC451.B47 2005

Physical chemistry : a molecular approach, McQuarrie, Donald A., University Science Books, c1997.
Call no: QD453.2 .C87 1997

Molecular quantum mechanics, Atkins, P. W., Oxford University Press, 2005.
Call no: QD462 .A85 2005, Online Resource Center: http://www.oup.com/uk/orc/bin/9780199274987/

Quantum chemistry, Levine, Ira N., 1937- Upper Saddle River, N.J. : Prentice Hall, c2000.
Call no: QD462 .L48 2009 (6th edition)

Fundamentals of physics, Halliday, D., Resnick R., Walker J.,John Wiley Sons Inc., 2008.
Call no: QC21.3 .H35 2005 (7th edition)

The chemistry maths book, Steiner, E., Oxford ; New York : Oxford University Press, 2008.
Call no: QA37.2 .S7985 (2nd edition)

Other resources:

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. **Mathcad is installed in all the computers in the chemistry computer lab**.

3. Contents

Weeks	Subjects Covered
(1-2)	**Time dependent quantum mechanics** Time dependent perturbation theory Interaction of radiation and matter Selection rules
(3-6)	**Chapter 13. Spectroscopy I: Rotational and Vibrational Spectra** **13.2.** The intensities of spectral lines **13.3.** Linewidths **13.4.** Moments of inertia **13.5.** The rotational energy levels **13.6.** Rotational transitions **13.7.** Rotational Raman spectra **13.9.** Molecular vibrations **13.10.** Selection rules **13.11.** Anharmonicity **13.12.** Vibration-rotation spectra **13.13.** Vibrational Raman spectra of diatomic molecules **13.14.** Normal modes **13.15.** Infrared absorption spectra of polyatomic molecules **13.16.** Vibrational Raman spectra of polyatomic molecules **13.17.** Symmetry aspects of molecular vibrations.
(7-9)	**Chapter 16. Statistical Thermodynamics 1: the concepts** **16.1.** Configurations and weights **16.2.** The molecular partition function **16.3.** The internal energy **16.4.** The statistical entropy **16.5.** The canonical ensemble **16.6.** The thermodynamic information in the partition function **16.7.** Independent molecules
(10-12)	**Chapter 17. Statistical Thermodynamics 2: applications** **17.1.** The thermodynamic functions **17.2.** The molecular partition function **17.3.** Mean energies **17.4.** Heat capacities **17.5.** Equations of state (briefly) **17.6.** Residual entropies **17.7.** Equilibrium constants
(13-14)	**Chapter 14. Spectroscopy II: electronic transitions** **14.1.** The electronic spectra of diatomic molecules **14.2.** The electronic spectra of polyatomic molecules **14.3.** Fluorescence and phosphorescence **14.4.** Dissociation and predissociation **14.5.** General principles of laser action **14.6.** Practical lasers (briefly) **14.7.** Application of lasers in chemistry **14.8-14.10.** Photoelectron spectroscopy
(15)	**Chapter 24. Molecular reaction dynamics*** **24.1.** Collision theory **24.2.** Diffusion-controlled reactions **24.3.** The material balance equation **24.4.** The Eyring equation **24.5.** Thermodynamic aspects **24.6.** Reactive collisions **24.7.** Potential energy surfaces **24.8.** Some results

* This material will be covered only if time permits.

4. Exams and Grading Policy

Midterm 1:	20%
Midterm 2:	20%
Quiz	10%
Homework:	10%
Final examination	40%

- All announcements (grades, assignments,…) will be posted on "METU-Class" website (and when possible via e-mail), and you are expected to check METU Online and METU e-mail accounts regularly (weekly).

5. 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 quoted the abovementioned academic integrity code.

***Code of Integrity ***
All students are expected to have academic integrity principle in all academic works. That is, a student must submit work only the student's own. Students shall comply with academic integrity codes and shall avoid situations likely to violate this code since academic dishonesty diminishes credit to the academic community.

Academic Dishonesty
Academic dishonesty is defined as any activity, which tends to undermine the academic integrity of the university. Academic integrity is one of the major factors that determines the image and dignity of the university. So not only academic people are responsible to maintain the duration of academic integrity, all members of the university including students should obey the rules and regulations of the university.

Academic Misconducts
Behaviour considered as misconduct or violation in academic terms are defined so:

a. Cheating

Cheating means giving or receiving any unauthorized aid in any academic exercise. It includes but is not limited to the following actions:
- *Copying from someone else's test or examination paper*
- *Using external assistance like the use of tutors, books, lecture notes and calculator in any in-class or take-home examination although it is prohibited*
- *Possessing, buying, selling, removing, receiving or using a copy or copies of any materials to be used as an instrument of academic evaluation*
- *Using another person as a substitute in an academic evaluation*
- *Working with other persons on a particular project although the instructor has required indivudial work*
- *Copying a report or homework assignment prepared by someone else or using records or laboratory results obtained by someone else as it is your work*
- *Attempting to influence or change any academic evaluation by unfair means which includes altering exam results or grades or changing anything on exam papers hiddenly while they are shown by the instructor for control and objections*

b. Plagiarism

Plagiarism means using a part or whole of a written material without proper acknowledgement of source. A student should pay attention to the originality of any material he or she uses for such situations:
- *Whenever he or she quotes another person's actual words,*
- *Paraphrases another person's words,*
- *Uses another person's idea, opinion or theory,*
- *Whenever he or she uses internet sources, borrows facts, statistics or any information which is not common knowledge.*
- *As a whole, theses, essays, term papers, and other academic project requirements must be the original work of the student who is submitting them. And while using other materials, the source should be properly and clearly defined by references.* For useful information regarding plagiarism check http://www.fbe.metu.edu.tr/Intihal/intihal.htm

3. Fabrication

Fabrication is defined as intentionally misrepresentation of any academic information or citation in order to deceive. A student must not falsify or invent any information or data in an academic exercise including, but not limited to, records or reports, laboratory results, and citations to the sources of information.

4. Interference
Interference is defined as trying to get advantage in any academic evaluation by unfair ways. This includes but is not limited to the following:

- *A student should not steal, change or destroy another student's work. This includes theft, defacement, harming or collecting all sources so as to prevent others to reach the information they contain.*
- *A student should not give or offer bribe, promise favors, make threats to any academic staff to change or affect any grade or result of any academic evaluation.*

5. Facilitating Academic Dishonesty

This means aiding or abetting others to cheat, to plagiarise or to commit any academic dishonesty. A student must not intentionally or knowingly help or attempt to help another student to commit an act of academic misconduct. It includes but is not limited to the following:

- *Giving unauthorized assistance to another or others during an academic evaluation like allowing students to copy from each other or lecture books or notes.*
- *Substituting for another student in an academic evaluation.*
- *Permitting one's academic work to be represented as the work of another.*
- *Providing any information about any academic evaluation before it takes place to a student such that that person gains an advantage for academic evaluation.*

6. Responsibility to Report Academic Dishonesty

Universities are academic entities which are devoted to innovate and transmit new knowledge for the scientific, technological, economic, cultural and social improvement of the society through scholarly research and related community services. The responsibility is to maintain an environment in which it members should behave in a good manner.

Academic Dishonesty is a serious threat to the dignity of the university. It decreases the quality of education and causes loss of confidence in terms of university premises. That's why it is the responsibility of all students to report any witnessed academic dishonesty. If one does not comply with university rules and regulations and academic misconducts stated above and if another one sees or realises this and does not report it to any academic unit, he or she will be a part of the violation committed against university's integrity.

* The parts in italic are adapted from the Instruction Technology Services Office website with minor modifications.

** The parts in italic are quoted from the METU Student Code of Conduct published by the METU Ethics Club.