

Chem 580 Molecular Structure and Spectroscopy Winter 2015

Professor Eitan Geva	e-mail eitan@umich.edu	Office Hour Upon request	Office 2000D Chem.
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Prerequisites:
Chem571 (or an equivalent course on quantum mechanics).

Website:
Lecture notes, problem sets, answer keys and announcements will be posted on the course CTools web site (<https://ctools.umich.edu/>).

Recommended textbook:
Detailed lecture notes will be provided, which can be used as a textbook.
The following book are also recommended as a reference:
“Principles of Nonlinear Optical Spectroscopy”, by Shaul Mukamel.

Class Schedule:
MWF 11:00 AM -12:00 PM Room 1636 Chem

Grading:
4 Problem Sets 200 pts. (50 pts. each).
Final Project 200 pts.
Total: 400 pts.

Problem Sets

Chem 580 students are **required** to submit 4 problem sets and a final project. Each problem set is worth 50 points. The final project will consist of writing a literature review or a research proposal related to the material covered in the course. **The problem sets will be posted on the web site.** The submission deadlines are given below:

Problem set #	Submission deadline
1	February 2
2	February 23
3	March 16
4	April 6
Final project	April 24

Problem sets must be prepared legibly with work shown in an orderly and logical manner. Explanations of your procedure should be given as needed to make clear what you have done. A specific numerical answer for each problem must be given with correct units and **highlighted (or enclosed in a box)**. Detailed answer keys will be posted on the CTools site following the submission deadline.

Tentative list of topics

- (0) **A survey of quantum chemistry**
- (1) **Quantum dynamics in Hilbert space.**
- (2) **Quantum dynamics in Liouville space.**
- (3) **Green function/operator techniques.**
- (4) **The quantum master equation.**
- (5) **Mixed quantum classical dynamics.**
- (6) **Electromagnetic radiation and radiation-matter interaction.**
- (7) **Optical response.**
- (8) **Optical response of a multi-level system governed by a quantum master equation.**
- (9) **Mixed quantum-classical approaches for calculating optical response tensors.**
- (10) **The Brownian oscillator model.**
- (11) **Pump-probe spectroscopy.**
- (12) **Fluorescence, Spontaneous-Raman and Coherent-Raman Spectroscopy.**