Chemistry 540 PRINCIPLES OF SPECTROSCOPY Fall 2021

Instructor: Piotr Piotrowiak, LSC 201D, tel. 973-353-3518, e-mail: *piotr@newark.rutgers.edu*
Class time & place: Monday, 6:00-9:00 PM, Smith Hall 242
Office hours: Thursday 10-12 and by appointment

Textbooks:
The primary reference material for the course will be *Quantum Chemistry and Spectroscopy* by Thomas Engel, ISBN-13: 978-0321766199; ISBN-10: 0321766199. We will supplement is as needed with excerpts from additional sources.

Objectives:
The course lays down the general theoretical groundwork necessary for the understanding of the interaction between electromagnetic radiation (light) and matter. Practical illustrations will be drawn primarily from electronic and vibrational spectroscopy, however, the main goal is to provide broad conceptual basis applicable to any type of spectroscopy, from routine UV-vis absorption to multidimensional NMR. The course begins with a review of undergraduate-level quantum mechanics and proceeds to introduce the concepts of transition probability, absorption, emission, dispersion, stimulated emission and laser action.

Grading:

1st midterm: October 11 – (a 30 minute in class quiz + a take home component) 15 %
Last date to drop with a grade of W: October 25
2nd midterm: November 22 – (a 30 minute in class quiz + a take home component) 15 %
Graded homework - 15%
Final: Date to be determined – (2 hours in class + an individual take home component) 55 %

Syllabus divided into major conceptual sections of the course:

1. September 8 (Wednesday) and 13 (Monday): Brief review of undergraduate level quantum mechanics including familiar solutions to the particle in the box, rigid rotor and harmonic oscillator. Orthogonality, normalization, eigenvalues, eigenfunctions, expectation values. Approximate methods of QM, i.e. the perturbation theory and the variational theorem.

2. September 20 and 27: The nature of electromagnetic radiation: Polarization of light, propagation through dispersive and absorptive media, interaction with charged particles. Phenomenological description of the absorption (Beer's law). Refraction. Maxwell's equations. Quantum mechanical aspects of electromagnetic radiation and corpuscular nature of photons.

3. October 4: Atomic level picture of the interaction between light and matter: The concept of a transition dipole. Transition dipole in rotational, vibrational and electronic spectroscopy. Black body radiation and quantization of absorption and emission of light. Einstein coefficients of absorption, spontaneous emission and stimulated emission. General principles of laser action.

4. October 11: Electronic spectroscopy: Born-Oppenheimer approximation and Franck-Condon factors. Discussing electronic transitions in terms of orbitals and states vs states. Selection rules. Excited states vs excitons – reconciling the language of spectroscopy in the molecular world and solid state materials (semiconductors).

5a. October 18: Intra- and inter-molecular non-radiative relaxation of electronic excited states. Internal conversion (IC), intersystem crossing (IST), vibrational redistribution and relaxation (IVR), conformational change, bond breaking and formation, conical intersections. Energy and electron transfer with examples of key photo-redox processes in living organisms, materials and catalysis.

5b. October 25 (Last date to drop the course with a grade of W): Förster model of energy transfer and Marcus theory of electron transfer with application. Concepts of reorganization energy and electronic coupling (super-exchange).

6. November 1: Time-resolved electronic and vibrational spectroscopy (pump-probe, upconversion, photon counting, etc.) including selected practical aspects of the relevant instrumentation and examples.

7. November 8 and 15: Time dependent approach to spectroscopy: Time-dependent perturbation theory. Coupling between the EM field and the transition dipole. Two-level system and the density matrix approach. Coherence and dephasing. Fermi's Golden Rule and transition probability. Oscillator strength and the QM expression for the emission rate. The fluctuation-dissipation theorem. Correlation functions and spectra as Fourier transform pairs. Coherence, photon echo, the rotating frame of reference. 2D spectroscopy (with examples from electronic, IR and NMR spectroscopy).

8. November 22: Non-linear optical spectroscopy. Harmonic generation, wave mixing, 2-photon processes, Kerr effect, their spectroscopic and diagnostic applications.

9. December 6: Elastic and inelastic light scattering. Raman scattering. X-ray scattering. Plasmon resonance.

10. December 12: Review of the material, distribution of the take-home assignments.

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https://ods.rutgers.edu/students/registration-form.