# Advanced Materials Characterization-Spring 22-23
# MAT 405 (Undergrad) / MAT 525 (Grad)

**Instructor:**
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**Assistants:**
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**Lecture hours and lecture rooms:**
- Monday 09:40-11:30, FENS G029 (MAT 405 / MAT 525)
- Monday 14:40-16:30, FENS L058 (MAT 405L)-**only for undergrads!**
- Thursday 17:40-18:30, FENS L055 (MAT 405 / MAT 525)

**Grading:**
- 1 Midterm %30, Date of midterm exam: TBA during the semester
- 1 Final %60, Date of final exam: TBA during the semester
- 1 Presentation %10, Date of presentation: TBA during the semester

**Participation:**
- Min. %70

**Office Hours:**
- By appointment

**References:**
- Atkin's Physical Chemistry, P. Atkins, Julio de Paula, 8th Edition

## DETAILED COURSE CONTENT:

### Part 1 (~2 Weeks)

1.1) Historical evolution of spectroscopy with classical and quantum physics phenomena
1.2) Electron and nuclear spin concepts, Stern-Gerlach experiment, importance of quantum numbers
1.3) Study of harmonic oscillator, rigid rotor, and particle in a box problem with Schrödinger equation
1.4) Importance of electromagnetic spectrum in spectroscopic methods
1.5) Introduction to magnetic resonance methods (Multiplicity, magnetic spin number, Pauli Principle, Hund's Rules, spectroscopic terms, Zeeman splitting)
1.6) Spin-Orbit Coupling, Spin-Hamiltonian, and energy terms (Zeeman, fine structure constant, hyperfine structure constant, crystal field parameters, quadrupole, g-factor), resonance condition
1.7) Ligand field theory, crystal field theory, identification of crystal field parameters with spectroscopic methods, crystal field stabilization energy (CFSE) calculations for octahedral and tetrahedral field symmetries in metal ions, calculation of orbital energies, CFSE calculations for more complex (less symmetric) fields
1.8) Introduction to metal complexes, absorption spectra of metal complexes, color wheel

### Part 2 (~3 or 4 Weeks)

2.1) Working principle of electron paramagnetic resonance (EPR) spectroscopy
2.2) Application and spectral analysis of EPR spectroscopy to semiconductor (ZnO), piezoelectric (PZT), and ferroelectric ($PbTiO_3$) materials, identification of point defect centers, and deduction of their concentrations. Comparison with photoluminescence spectroscopic method and extraction of defect structure models of semiconductor materials by complementary spectroscopic methods of EPR, Photoluminescence, UV-VIS, which will form the basis of bandgap engineering (Tauc formula, Bruss formula)
2.3) Application of EPR spectroscopy to solar cells, superconductors
2.4) Some basics of semiconductors and their relation to EPR spectroscopy via defects

**Part 3 (~2 or 3 Weeks)**
3.1) Introduction to Nuclear Magnetic Resonance (NMR) spectroscopy, angular momentum concept and nuclear magnetism
3.2) Behavior of hydrogen atom in magnetic field
3.3) Shielding effect in NMR spectroscopy, resonance condition, gyromagnetic ratio constant, chemical shift
3.4) Working principle of NMR spectroscopy
3.5) Difference between liquid and solid-state NMR
3.6) Identification of molecules containing carbon and hydrogen in NMR spectra
3.7) Why is TMS molecule used as a reference in NMR?, Calculation of ppm from Hz
3.8) Special methods for solid-state NMR (magic angle spinning, cross polarization, special 2D methods)
3.9) Differences in NMR rotors, varieties, and applications
3.10) Application of NMR spectroscopy in biological materials

**Part 4 (~1 Week)**
4.1) Historical evolution of Atomic Force Microscopy (AFM) and working principle of AFM
4.2) Detailed analysis of AFM operation modes (contact mode, non-contact mode, tapping mode), advantages and disadvantages of these modes

**Part 5 (~2 Weeks)**
5.1) Introduction to Dynamic Light Scattering (DLS) method, What is scattering?, Turbidity concept
5.2) Differences between static and dynamic light scattering
5.3) Study of limits in DLS method
5.4) Stokes-Einstein equation, particle size and hydrodynamic size, differences between results obtained from TEM and DLS
5.5) How to obtain particle size from DLS?, detailed auto-correlation process

**Part 6 (~1 Week)**
6.1) Introduction to impedance spectroscopy
6.2) AC/DC current, Voltage-time graphs, and their meanings
6.3) Resistance and impedance definitions, Ohmic, and non-Ohmic behavior
6.4) Series and parallel RLC circuit, Nyquist and Cole-Cole Plots, and their meanings, Randles circuit
6.5) Capacitor, inductor circuit elements
6.6) How to take impedance measurements? e.g., Supercapacitors (design and test)

**Part 7 (~1 or 2 Weeks)**
Student's presentations

**MAT 405L - Advanced Materials Characterization Lab (only for undergrads!)**
Students could make measurements with the spectroscopic, scattering, and microscopic techniques described. Meanwhile, the simulation of spectra obtained by spectroscopic methods with the help of the MATLAB and modeling of materials, especially defect structures, are in the content of the laboratory section.

Accordingly, the following demos will be carried out:
1) Using EPR spectroscopy and calculating the EPR spectra of a prototype semiconductor material such as ZnO, determining the defect centers,
2) Measurement of Mn metal ion-doped ZnO samples by EPR
3) Extraction and interpretation of Spin-Hamiltonian parameters by simulating the measured spectra by writing codes in the MATLAB
4) Utilizing NMR spectroscopy and obtaining H spectra of various molecules
5) Defining the DLS technique to the students practice in the DLS lab
6) Introducing the AFM technique to the students in the AFM lab.
7) Performance tests of supercapacitors designed by students using impedance spectroscopy technique