CHEM 3031 Physical Inorganic Chemistry 2014

Office hour: TBD CB456
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Website: www.moodle.yorku.ca

Course Outline:

1. Introduction and survey of spectroscopic techniques for inorganic chemistry: NMR, ESR, IR, Raman, Mass-Spec, XPS/UPS and CD.
2. Symmetry and Group theory.
3. Molecular orbital theory of diatomic, polyatomic and organometallic complexes. LCAO, angular overlap approximation, sigma/pi interactions, lability of complexes and hard-soft acid-base concept.
4. One-dimensional materials: Peierl's distortion, MLCT and redox chemistry.
5. Materials/Solid state chemistry - Band theory, electronic properties, phase diagrams, synthesis, and introduction to nanochemistry.

Learning Objectives:

Spectroscopy. Students are taught the basics of spectroscopic techniques that are used to characterize inorganic complexes. This course prepares students to:

1. Describe and understand the working principle of different spectroscopic techniques
2. Predict the NMR and ESR spectra of inorganic complexes containing nuclei of different spins
3. Identify the structure of inorganic compounds through a combination of magnetic resonance, vibrational, optical and photoelectron spectroscopies.

Symmetry, Group Theory and MO Theory. Students are taught more advanced knowledge of symmetry, group theory and MO theory. This course prepares students to:

1. Apply symmetry operations to identify the point group of the compound
2. Generate irreducible representations that are used to predict the IR and Raman vibrational modes
3. Derive MOs of diatomic, polyatomic and coordination complexes based on symmetry-adapted linear-combination of atomic orbitals
4. Explain how sigma and pi interactions affect MO
5. Use angular-overlap approximation to predict the relative energies of the MO and lability of ligands
6. Apply frontier orbital theory to explain chemical reactivity
7. Understand hard-soft acid-base theory based on frontier MOs
8. Case studies of inorganic complexes for electrocatalysis and solar energy conversion

Materials and Solid State Chemistry. Students are introduced to one-dimensional inorganic compounds, bulk solid state materials and nanostructures. This course prepares students to:

1. Describe and understand the bonding of 1D chain-like structures using MO theory and Peierl's distortion
2. Analyze band theory from atomic orbitals and MO perspectives
3. Describe and understand redox chemistry of selected compounds
4. Explain electronic properties of 1D materials (glyoximate/pthalocyanine complexes, Krogmann's salt, Wolfram's salt), 2D material (graphite), semiconductor, metal, semimetal and insulator
5. Understand the effect of dopants on the electronic properties of semiconductors and their technological applications

6. Describe the synthesis of solid state materials and their crystal structures including perovskite and magnetite
7. Understand and apply phase diagrams for the growth of single crystals
8. Describe the chemistry and properties of exemplary nanomaterials