Course Title: Chemistry 3210: Materials Chemistry

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office: 5014 (not that this really matters these days)

Traditionally, I have an open-door policy, which means I normally don't have office hourse. This is obviously a bit more challenging with the pandemic, so I will have office hours on Thursday from 10-11. If that time doesn't work out, then I am more than happy to arrange other times to meet. If you have questions about a topic, then we can arrange a time to meet via webex. If a group of you have some questions about a topic, then we can arrange a time to meet via webex. My goal is to help in any way possible.

Asking questions is one of the most important things that you can do in any course. I encourage you to ask me questions as often as possible. I also encourage you to ask yourself questions, and then try to come up with answers; just ask yourself if your answers make sense too.

I am more than happy to help with your assignments/labs/questions or any course or research-related question.

Please do not hesitate to ask questions. You will never do worse in a course for asking questions.

Strongly-Recommended Text:

There are lots of great texts available for materials chemistry. I am a fan of West's books. I find them easy to understand. I will do my best to link the topics we are covering in the course with chapters in various books/online resources.

- Inorganic Chemistry 6th Edition by Shriver, Weller, Overton, Rourke, Armstrong
  - This is a good general inorganic chemistry book.
- Basic Solid-State Chemistry 2nd Edition by West
  - This is the book that I use to develop the course and the book that I used when I was a student (somehow I now have 2 copies of the book)
- Solid-State Chemistry and its applications 2nd edition by West
  - This is a more modern textbook whose PDF may be available.

General Course Description: A detailed examination of the structure-property relationships and their applications to materials science.

Course Information:

The course focuses on examining the solid state. In solution, physical properties are governed by the molecule. However, in the solid-state, the physical properties are governed by how molecules are arranged relative to one another. The course will introduce the basics of structure as well as some common structure types. We will then examine bonding in solids and how the properties of a material can be due to "errors" in the structure. We will then examine phase diagrams of binary materials to determine what reactivity two species will have with one another (synthetic chemistry for solids).

Topics:

0. Introduction (1 lecture)
   a. What is materials chemistry?
1. Structure (approximately 8-10 lectures)
   a. Unit-cells
      i. 1.1 + 1.3 (solid-state chem and applications)
   b. Bravais Lattice (symmetry)
      i. 1.4
   c. Lattice planes, Miller Indices, indices of directions
      i. 1.5

        ii. I also created a javascript-based program to explore Lattice planes www.KatzResearchGroup.com/Miller.html
            1. I'm always looking for feedback and suggestions on this and potential new demonstrations that will help with the class, so don't hesitate to reach out with suggestions.
    d. d-spacing
        i. 1.6-1.7
    e. Interactions of x-rays with crystalline solids
        i. Chapter 5 (5.3.2 , 5.3.4.2, 5.3.6.5-5.3.6.6 and some of 5.3.7)
            1. This topic is extensive, and I could teach a whole class just on X-ray diffraction, but I want to give you the bare necessities of what you will need.
    f. Crystal density and unit cell contents
        i. 1.8
    g. Close-packed structures (and non-closed packed structures?)
        i. 1.15
        ii. I also created a javascript-based program to explore Lattice planes www.KatzResearchGroup.com/ClosedPacked.html
            1. I'm always looking for feedback and suggestions on this and potential new demonstrations that will help with the class, so don't hesitate to reach out with suggestions.
    h. Unit cell projections
        i. 1.14
    i. Different structure types
        i. 1.15
2. Property
    a. Bonding
        i. 3.4
    b. Band theory (3-4 lectures)
        i. Conductivity
        ii. Semi-conductivity
        iii. Solar-energy conversion
    c. Crystal Defects/dopants (4-5 lectures)
        i. Chapter 2
    d. Phase diagrams (4 lectures)
        i. Chapter 7
    e. Nuclear Science (?)
        i. Time dependent
    f. Magnetism (3 lectures)
        i. Some of Chapter 9
    g. Superconductivity (1 lecture)
        i. 8.3 (briefly)
    h. Pyroelectricity, ferroelectricity, piezoelectricity (1 lecture)
        i. 8.6-8.10 (briefly)

Method of Evaluation:

Topics:

Grading:

1. **Assignments** **20 %**
    a. I will give you some assignments during the course to help you with the course material. The aim is for these to be small assignments to help you keep on top of the topics.
2. **Take home Midterms (2 midterms)** **20 %**
    a. This will cover all of Structure
    b. This will cover properties, but not all of them (Ideally including phase diagram but it may not).
3. **Lab** **30 %**
    a. There will be 4-6 labs that will be like larger assignments. This will have you digging in a bit further into a course topic than a typical assignment.
        i. Lab 1: X-ray diffraction analysis
        ii. Lab 2: structure exploring
            1. You will use a software package called Mercury that is free to use to look at structure files. Mercury is written by the Cambridge crystallographic data centre (CCDC). If you install it ahead of time, then please note that you have to go into the software activation program and go to "Active CSD-community" tab and then activate the free version. Do not purchase a licence for this. This is expensive and unnecessary.
                a. There are other programs as well if you are interested
                    i. Gavrog, VESTA, crystal impact
        iii. Lab 3: Solar energy and band structure
        iv. Lab 4: Phase diagram lab
        v. Lab 5: critique a materials chemistry paper
4. **Final Assignment** **30 %**
    This will be a final project on a topic from the course. Here are some potential topics. I will make a more exhaustive list on D2L as we get further into the course
        1. Quasi-crystals
        2. Dye-sensitized solar cells (DSSCs)
        3. Solar energy conversion (not DSSCs)
        4. Solar fuels
        5. Piezoelectrics
        6. Ferroelectrics
        7. Spin frustration (magnetism)
        8. other

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Regulations, could be construed as dishonest or improper. Students found guilty of an academic offence may be subject to a number of penalties commensurate with the offence including reprimand, reduction of grade, probation, suspension or expulsion from the University. For more information regarding this policy, students should refer to the
University Regulations for Academic Misconduct (Section 6.12) in the University Calendar.

Academic misconduct information can be found at http://www.mun.ca/regoff/calendar/sectionNo=REGS-0748.
http://www.library.mun.ca/researchtools/guides/integrity/