

## MATRL 218/CHEM 277: Introduction to Inorganic Materials

### Catalog Description:

An introduction to typical inorganic materials, with an emphasis on crystalline materials (some discussion of quasicrystalline and amorphous materials) and how their material properties can be understood based on the constituent atoms, and the crystal and electronic structure. Includes rudiments of crystallography, and notions of how crystal structures are built up from the concepts of close-packing and of the linking of polyhedra. Some discussion of specific structure types with reference to advanced material properties such as superconductivity, ferroic behavior and magnetism.

### Target audience:

The course is for graduate students with some prior knowledge of inorganic materials and crystallography. Advanced undergraduate students are welcome.

### Textbooks (none are required):

Properties of Materials: Anisotropy, Symmetry, Structure, R. E. Newnham, Oxford, 2004. ISBN-10: 019852076X, ISBN-13: 978-0198520764

The Basics of Crystallography and Diffraction, C. Hammond, Oxford-IUCr, 1997. ISBN 0-19-855945-3

Structure and Dynamics: An Atomic View of Materials, M. T. Dove, Oxford, 2003. ISBN: 0-198-50678-3

Electronic Structure and Chemistry of Solids, P. A. Cox, Oxford University Press, 1987. ISBN 0-19-855204-1

Inorganic Structural Chemistry, U. Müller, John Wiley, 1993. ISBN 0-471-93717-7

Crystal structures: A Working Approach, H. D. Megaw, W. B. Saunders, 1973. ISBN 0-721-66260-9

### Instructor:

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### Grader:

Phillip Barton

### Course Website:

<http://www.mrl.ucsb.edu/~seshadri/teach.html>

### Grading:

4 best from 5/6 assignments (20%), midterm (30%), take-home final (50%).

**Outline:**

1. Why understand structure-property relationships?
2. Classification of materials as amorphous and crystalline, and the structural hierarchy in a polycrystalline material. Quasicrystalline and amorphous materials. The glass transition.
3. Cohesion in solids Ionic, covalent, metallic, van der Waals
4. Crystallography in a nutshell: Lattices, unit cells, symmetry how crystallography simplifies the depiction of structures
5. Packings: CCP and HCP, voids, radius ratio rules, the structures of elements –  $\alpha$ -Po, Fe, Cu, Mg, Si, C (graphite)
6. Paulings rules for ionic crystals and the concept of Bond Valence
7. Description of crystal structures: AB, AB<sub>2</sub>, AB<sub>3</sub> (ReO<sub>3</sub>), perovskites, K<sub>2</sub>NiF<sub>4</sub>
8. Electronic structures of crystalline solids – energy bands, densities of states, crystal fields, the band gaps in semiconductors
9. Metals, non-metals and the metal-insulator transitions examples of perovskites
10. Cooperative magnetism in solids – examples of perovskites and spinels
11. Structural phase transitions in solids – the example of BaTiO<sub>3</sub>
12. Special topics: Structure-property relations in advanced materials:
  - (a) GMR/CMR: Systems and phenomena
  - (b) Polar materials: Normal and relaxor ferroelectrics, and piezoelectric materials High  $T_C$  superconductors