EMS 289C
Structure and Thermodynamics of Materials
Winter 2019
Tuesday and Thursday 1^{30}- 3 pm
Chem Annex 4440
CRN# 32940
Register for 3 credits

Prof. Alexandra Navrotsky
Phone752-3292
anavrotsky@ucdavis.edu

This materials science course is aimed at graduate students in *materials science, chemical engineering, chemistry, physics, geology, environmental science, and related fields*. Its purpose is to give an overview of the structure, thermodynamics, and properties of inorganic materials, with an emphasis on oxides and silicates and some discussion of nitrides and hybrid materials. The relations among fundamental structural features (local coordination and polyhedral linkages) , thermodynamics, and other properties will be stressed, as will the relations among different structures. Crystalline, disordered, amorphous, and nanophase materials will be discussed. Applications range from ceramics to nanomaterials to glasses and to energy to environmental science and geochemistry . Applications to nuclear materials will also be presented and this course qualifies for DENS, the Designated Emphasis in Nuclear Science.

This course is strongly recommended for materials science first and second year students and for those chemical engineers who may work at all on solids. It is similar to the solid state chemistry course I sometimes teach through the chemistry department and chemistry students are especially encouraged to participate. It could count, with your advisor's permission, as a *chemistry elective*.

A suggested book, old but still useful, is "Physics and Chemistry of Earth Materials", A. Navrotsky, Cambridge Univ. Press (1994) (which you can get through Amazon). In addition you can access various modern crystallographic software via the internet. You will be expected to go to other books and original research papers for specific information. Grading will be on the basis of three problem sets and a 20 minute in-class presentation.

Ceramic and electronic materials are largely inorganic solids. Minerals are natural solid state materials, primarily silicates, oxides, sulfides, halides, and metals. This series of lectures will examine the structure, bonding, stability, and properties of solids from the viewpoint of modern physics, chemistry, and materials science. Necessary fundamental concepts related to crystallography, spectroscopy, crystal chemistry, and thermodynamics will be reviewed briefly. Applications to specific materials will be integrated into all course activities.

Topics to be covered

1. Fundamental of symmetry, crystallographic nomenclature, and crystal structure determination: a brief review.
2. Description of structure types:
    - Elements (metals and nonmetals)
    - AX compounds (including semiconductors)
    - AX_2, AX_3, and A_2X_3 compounds
    - ABX_3 and AB_2X_4 compounds
    - Complex structures (alloys, ceramics, silicates, minerals)
    - Organic and hybrid materials
3. Fundamental questions and relations:
    - "Why" a particular structure
    - Concepts of size, bond type, etc.
    - Families of related structures and order-disorder
    - Relating structure and thermodynamics
    - Structure property relations
4. Means of studying structures of solids:
    - Diffraction techniques (X-ray, neutron)
    - Electron microscopy
    - Vibrational spectroscopy, (IR, Raman)
    - NMR
    - Spectroscopic probes of electronic states
    - Uses of synchrotron radiation
    - Computational approaches
5. Thermodynamics of solids
    - Basic principles
    - Phase transitions
    - Solid solutions
    - Phase diagrams
    - Experimental methods, especially calorimetry
    - Computational approaches