Syllabus
EAS 6221 - Mineral Surface Geochemistry

3 credit hours.
No required textbook. (See "helpful references" section.)

Course Summary: Interactions of aqueous solutions with the surface of minerals and particles with emphasis on structure, sorption processes, crystal growth and dissolution processes, and biomineralization reactions.

Format: This course is composed of lectures, (almost) weekly exercises, and a paper with presentation to the class. The paper and presentation should be on current (or nearly current) research dealing with mineral surface structure and reactivity. This can be drawn from your own research, but please try to stay on topic. Grades will be determined by the following ratio:

item:	percentage of grade:
class participation	5
exercises	65
paper	20
presentation	10

Notice that class participation is a significant portion of the grade. To do well in this category, it is recommended to attend class as much as physically possible, read the reading assignments, and participate in class discussions or answer questions that I pose to the class.

Course material:
Background Chemistry
- Phases of matter
- Define mineral and importance of mineral surfaces
- Packing of atoms
- Interactions between atoms
  - Types of bonds
  - Pauling's rules for bonding
  - Molecular and atomic orbitals

Background Mineralogy
- space groups and symmetry
- classification by anion
- silicate structure and classification
- determination of structure: X-ray diffraction

Surface structure
- concept of most energetically favorable termination
- in vacuo terminations
- in situ terminations
- determination of structure
  - X-ray photoelectron spectroscopy
  - Auger electron spectroscopy
  - X-ray absorption spectroscopy fine structure
  - crystal truncation rod

Adsorption

- Thermodynamic driving force
- isotherms
- dissociative adsorption of water
- surface charge
- surface complexation modeling
  - constant capacitance
  - diffuse layer
  - triple and four-layer
- surface complexation measurement
  - batch adsorption
  - crystal truncation rod
  - cation versus anion adsorption
- cation and anion exchange capacities

Crystal growth and dissolution
- bulk kinetic measurements
  - rate models
  - surface area measurement (Brunauer, Emmet, Teller isotherm)
  - why (most) rate models are wrong
- Burton, Cabrera, Frank theory (a.k.a. cubonium)
- modern classical crystal growth theory
- dissolution as a ligand exchange

Electrochemical reactions at surfaces
- concept of electrode potential
- Band theory
- Marcus theory
- photochemistry
- oxidative and reductive dissolution

Biomineralization and growth inhibition
- methods of influencing growth morphology
- kinetic models of growth inhibition

Colloids and nanoparticles
- structure and synthesis
- reactivity

(if time) Computational techniques
- monte carlo
- molecular dynamics
- ab initio

(if time) Microbes and minerals
- sulfide oxidation
- dissolution of iron (oxy)(hydr)oxides
  - assimilation
  - dissimilation
- precipitation
- models, or lack thereof

Honor Code:
Students in this class are expected to abide by the Georgia Tech Honor Code and avoid any instances of academic misconduct, including but not limited to:

1. Possessing, using, or exchanging improperly acquired written or oral information in the preparation of a paper or for an exam.
2. Substitution of material that is wholly or substantially identical to that created or published by another individual or individuals.
3. False claims of performance or work that has been submitted by the student.

Helpful References:

General Geochemistry
Drever, J. I. (1997) The Geochemistry of Natural Waters: Surface and Groundwater Environments. Prentice Hall, New Jersey.
Spectroscopic techniques (XPS, AES), Surface structure
Hochella, M. F. Jr. (1990) Reviews in Mineralogy, Vol. 23, pages 87-132.
Surface charge and surface complexation modeling
Parks, G. A. (1990) Reviews in Mineralogy, Vol. 23, pages 133-176.
Davis, J. A.; Kent, D. B. (1990) Rev. Mineral., Vol. 23, pages 177-260.
EXAFS
Brown, G. E., Jr. (1990) Rev. Mineral., Vol. 23, pages 309-364.
Crystal Growth
De Yoreo, J. J.; Vekilov, P. G. (2003) Rev. Mineral. Geochem., Vol. 54, 57-94.
Biomineralization
Weiner, S.; Dove, P. M. (2003) Rev. Mineral. Geochem., Vol. 54, 1-30.
Ligand Exchange
Casey, W. H.; Ludwig, C. (1995) Rev. Mineral., Vol. 31, 87-118.
Points of Zero Charge
Sahai N. and Sverjensky D. A. (1997) Geochim. Cosmochim. Acta 61, 2801–2826.
Minerals as semiconductors
Xu, Y.; Schoonen, A. A. (2000) Am. Mineral., Vol. 85, 543-556.
Marcus Theory
Grätzel, M. (1989) Heterogeneous Photochemical Electron Transfer. CRC Press, Inc. Boca Raton, FL, pages 1-42.
Computational techniques
Foreseman, J. B.; Frisch, Æ (1993) Exploring Chemistry with Electronic Structure Methods. Gaussian, Inc. Pittsburgh, PA, pages 1-12.
Cygan, R. (2001) Rev. Mineral. Geochem., Vol. 42, pages 1-36.