ENVIRONMENTAL WATER CHEMISTRY (**CHE-100) Winter, 2019;**
1:40 - 3:00 pm. 215 Haring Hall

DESCRIPTION: The course covers practical aspects of water chemistry including thermodynamic relations, coordination chemistry, solubility calculations, redox reactions and rate laws. Laboratory assignments include determination of solute concentrations in natural waters and computer modeling of the evolution in water chemistry that follows from contact with minerals and gases.

COURSE and LEARNING GOALS: To instruct undergraduate students in the use of thermodynamics and molecular concepts to solve contemporary problems in water chemistry. Students are expected to demonstrate a working knowledge of the concepts in examinations and to complete a final project that involves computer simulation of natural water chemistry and knowledgeable interpretation of the results.

TEXT: '*Water Chemistry*' by Snoeyink and Jenkins is augmented with readings from case studies. The VMinteq computer programs is free and is used extensively. It can be downloaded for free from: http://www.lwr.kth.se/English/OurSoftware/vminteq/ The book relies upon this program.

ENTRY LEVEL: CHE 2-B.

OFFICE HOURS: Office Hours immediately after class; in 1480 Chem. Annex.

COURSE FORMAT: Three hours of lecture per week with weekly homework sets and exercises that reinforce lecture information.

COURSE GRADING: Grades are based upon homework sets and exercises (20%), two mid-term examinations (25% each; 50% total), the final project, which is treated as a final exam (30%). The tests are comprehensive.

Students are assumed to be knowledgeable about the UCD policies on Academic Integrity (see: http://sja.ucdavis.edu/academic-integrity.html). Students are required to turn in their own work, unless otherwise noted by Prof. Casey; plagiarism and cheating are referred to Student Judicial Affairs for investigation and adjudication. Please familiarize yourself with the UCD Policy on Academic Integrity.

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TOPICAL OUTLINE:

1) Constraining Equations and Water Analyses
    1.1 Thermodynamics of electrolyte solutions; saturation states
    1.2 Concentration scales
    1.3 Sampling natural waters
    1.4 Assessing analytical accuracy
    1.5 Common minerals in the shallow Earth that affect waters

2) Speciation via Acid-Base Equilibria
    2.1 The constraining equations for thermodynamic analysis
    2.2 Conjugate acid/base combinations
    2.3 Natural ampholytes
    2.4 Ion-pairing and complexation
    2.5 Species predominance diagrams

3) Carbonate Equilibria and Gases Exchange in Nature
    3.1 Volatile components in nature
    3.2 Calculations for closed- and open systems

3.3 Equilibrium with carbonate minerals
3.4 **Case Study**: Catastrophic CO_2 loss from Lake Nyos, Cameroon
3.5 Buffer intensity calculations introduced.

4) Hydrolysis Equilibria and Mineral Formation
    4.1 Source of metals
    4.2 Hydrolysis diagrams to elucidate open-system calculations
    4.3 Solubility of solid hydroxide and oxide minerals in the Earth
    4.4 Reactivity trends in oxides and oxyanions.
    4.5 Natural pH buffering and buffer-intensity calculations

Exam #1: tentatively January 24, 2018

5) Coordination Chemistry and Solution Electrostatics
    5.1 Natural and anthropogenic chelating agents
    5.2 Outer-sphere ion pairs--the Fuoss Equation
    5.3 Activity-coefficient corrections
    5.4 Gouy-Chapman theory of electrified solids
    5.5 Natural ion-exchanging materials

6) Reaction-path modeling and Case Studies
    6.1 Seawater
    6.2 Metal pollution of the River Glatt
    6.3 Alkali lake chemistry in the western U.S.
    6.4 Reaction-Path calculations via NetPath software

7) Redox Equilibria/Disequilibria
    7.1 The relative stabilities of sulfides, oxides, carbonates and molecular salts
    7.2 Electron-exchange rates in organic-poor natural waters
    7.3 Catalysis by microbes in organic-rich environments
    7.4 pH and pe as Master Variables

Exam #2: tentatively February 21, 2018

8) **Case Studies**: Redox disequilibria and the failure of equilibrium modeling
    8.1 The Fenton Reaction and pollutant oxidation in the atmosphere
    8.2 The Lindberg/Runnells study of U.S. groundwaters
    8.3 Redox reactions in hydrocarbon-polluted environments.

9) **Case Studies:** Challenges to this generation of chemists and geochemists:
    9.1 Actinide pollution at the Hanford Reservation, USA and at the Techa River, Chelyabinsk facility
    9.2 Pharmaceuticals in water
    9.3 Abiotic pesticide degradation pathways
    9.4 The *Biotic Ligand Model* of ecosystem toxicology

10) Final Exam--thermodynamic simulation of the returned water analyses.