

# EPSc 511: Minerals in Aqueous Environments

3 Credits

**Instructor:** Prof. Jeff Catalano, Rudolph Hall 242, 935-6015, [catalano@wustl.edu](mailto:catalano@wustl.edu)

**Meeting Times and Place:** T-Th 8:30 to 10 am, Rudolph Hall 204

**Course Website:** <http://epsc511.wustl.edu/>

## Course Objectives:

- To understand the common minerals that occur in low-temperature aqueous systems and the processes that control their reactivity and stability.
- To become familiar with analytical methods frequently used in aqueous geochemistry and mineralogy.
- To effectively read and critically review scientific literature.

**Course Description:** Coordination chemistry, chemical bonding, and the nature of water and aqueous solutions. Systematic mineralogy and crystal chemistry of common low-temperature minerals, including clays, zeolites, carbonates, phosphates, sulfates, oxides of aluminum, iron and manganese, and metal sulfides. Reactions between minerals and aqueous solutions, including growth and dissolution, surface complexation, and redox reactions. Properties of water and aqueous solutions. Role of mineral surface reactions in chemical weathering of silicates and carbonates, clay formation, microbe-mineral interactions, and nanoparticle behavior. Focus is on understanding mineral-water interface processes and mechanisms at the molecular level. Common analytical methods used in mineral-water interface studies will be introduced throughout the course.

**Reading Material:** There is no assigned textbook. Handouts and papers will be provided throughout the semester as reading assignments. To save paper, materials available over the internet will be linked to on the course website instead of being handed out in print.

A number of books will serve as useful references for this course. It is important that every student has access to a mineralogy textbook and an aqueous geochemistry textbook. The following are suggested (Note: The second title is available online through our library):

- *Manual of Mineral Science*, 23<sup>rd</sup> edition, by Cornelis Klein and Barbara Dutrow
- *Geochemistry, Groundwater, and Pollution*, 2<sup>nd</sup> edition, by C.A.J. Appelo and D. Postma

Additional useful reference books include:

- *The Surface Chemistry of Natural Particles*, by Garrison Sposito
- *Mineralogical Applications of Crystal Field Theory*, by Roger G. Burns
- *Physics and Chemistry of Earth Materials*, by Alexandra Navrotsky
- *X-ray Diffraction and the Identification and Analysis of Clay Minerals*, 2<sup>nd</sup> edition, by Duane M. Moore, Robert C. Reynolds, Jr.
- *Kinetics of Water-Rock Interaction*, by Susan L. Brantley, James D. Kubicki, Art F. White

- *Geochemical Rate Models*, by J. Donald Rimdstidt
- *Introduction to Geomicrobiology*, by Kurt Konhauser
- *Methods of Soil Analysis - Part 5: Mineralogical Methods*, by L.R. Drees, A.L. Ulery
- *Soil Mineralogy with Environmental Applications*, by Joe B. Dixon and Darrell G. Schulze
- Many volumes of *Reviews in Mineralogy/Reviews in Mineralogy and Geochemistry*

**Course Responsibilities:** Course grades will be determined based on homework assignments and two presentation and paper projects:

**Assignments (35%):** Students will be assigned five assignments during the semester. These will include problem sets dealing with chemical bonding and mineral structure as well as writing activities, including critical reviews and a short proposal to use an instrument as part of a research project.

**Project 1 (25%):** Students will select a mineral or class of minerals relevant to low-temperature geochemical systems. Each student will prepare a ~20 minute presentation and a 6-12 page paper reviewing the structure, occurrence, formation, and chemical properties of this mineral.

**Project 2 (40%):** Students will select a topic of interest not covered in detail in the class in consultation with the instructor. Each student will prepare a 15-20 page paper reviewing that topic.

**Academic Integrity:** All students are expected to adhere to high standards of academic integrity as outlined in our academic integrity policies:

Undergraduate Students: <http://wustl.edu/policies/undergraduate-academic-integrity.html>

Graduate Students: <https://graduateschool.wustl.edu/policies-procedures>

It is the responsibility of each student to read and be familiar with these policies. Unfamiliarity because of failure to read the respective document is not an excuse for lack of compliance. If you have any doubts or questions about the policies, please ask the instructor.

**Academic Accommodations:**

**Disability Resources** - At Washington University we strive to make the academic experience accessible and inclusive. If you anticipate or experience barriers based on disability, please contact Disability Resources at 314.935.5970, [disabilityresources@wustl.edu](mailto:disabilityresources@wustl.edu), or visit our website for information about requesting academic accommodations. See: <https://students.wustl.edu/disability-resources/>

**Sexual Assault Resources** - The University is committed to offering reasonable academic accommodations (e.g., no contact order, course changes) to students who are victims of relationship or sexual violence, regardless of whether they seek criminal or disciplinary action. If you need to request such accommodations, please contact the Relationship and Sexual Violence Prevention Center (RSVP) at [rsvpcenter@wustl.edu](mailto:rsvpcenter@wustl.edu) or 314-935-3445 to schedule an appointment with an RSVP confidential, licensed counselor. Information shared with counselors is confidential. However, requests for accommodations will be coordinated

with the appropriate University administrators and faculty. See: <https://students.wustl.edu/relationship-sexual-violence-prevention-center/>.

### **Reporting Sexual Assault:**

If a student discusses or discloses an instance of sexual assault, sex discrimination, sexual harassment, dating violence, domestic violence or stalking, or if a faculty member otherwise observes or becomes aware of such an allegation, they will keep the information as private as possible, but as a faculty member of Washington University, they are required to immediately report it to the Department Chair or Dean or directly to Ms. Jessica Kennedy, the University's Title IX Director, at (314) 935-3118, [jwkennedy@wustl.edu](mailto:jwkennedy@wustl.edu). Additionally, you can report incidents or complaints to the Office of Student Conduct and Community Standards or by contacting WUPD at (314) 935-5555 or your local law enforcement agency. See: <https://titleix.wustl.edu/>.

### **Bias Reporting:**

The University has a process through which students, faculty, staff and community members who have experienced or witnessed incidents of bias, prejudice or discrimination against a student can report their experiences to the University's Bias Report and Support System (BRSS) team. See: <https://students.wustl.edu/bias-report-support-system/>.

### **Mental Health:**

Mental Health Services' professional staff members work with students to resolve personal and interpersonal difficulties, many of which can affect the academic experience. These include conflicts with or worry about friends or family, concerns about eating or drinking patterns, and feelings of anxiety and depression. See: <https://students.wustl.edu/mental-health-services/>.

### **Center for Diversity and Inclusion (CDI):**

The Center for Diversity and Inclusion (CDI) supports and advocates for undergraduate, graduate, and professional school students from underrepresented and/or marginalized populations, collaborates with campus and community partners, and promotes dialogue and social change to cultivate and foster a supportive campus climate for students of all backgrounds, cultures and identities. See: <https://diversityinclusion.wustl.edu/>.

### **Preferred Name and Gender Inclusive Pronouns:**

In order to affirm each person's gender identity and lived experiences, it is important that we ask and check in with others about pronouns. This simple effort can make a profound difference in a person's experience of safety, respect, and support. See: <https://students.wustl.edu/gender-pronouns-information/>, <https://registrar.wustl.edu/student-records/ssn-name-changes/preferred-name/>.

### **Military Service Leave:**

Washington University recognizes that students serving in the U.S. Armed Forces and their family members may encounter situations where military service forces them to withdraw from a course of study, sometimes with little notice. Students may contact the Office of Military and Veteran Services at (314) 935-2609 or [veterans@wustl.edu](mailto:veterans@wustl.edu) and their academic dean for guidance and assistance. See: <https://veterans.wustl.edu/policies/policy-for-military-students/>.

**Course Schedule:** Listed below is a tentative schedule. All readings will be announced in class.

<b>Date</b>	<b>Topic</b>
<b>1/14</b>	<b>NO CLASS: Prof. Catalano at Geobiology Gordon Conference</b>
1/16	Introduction: Course Overview, Properties of Atoms and Molecules, Chemical Bonding
1/21	Coordination Chemistry: Pauling's Rules, Electroneutrality Principle, Bond Valences, Ion Coordination in Water
1/23	Transition Metal Chemistry: Crystal Field/Molecular Orbital Theories
1/28	Review of Mineralogy and Crystallography; Methods: Introduction to Powder X-ray Diffraction
1/30	Methods: Introduction to Powder X-ray Diffraction; Minerals: Rock-forming Silicates, Phyllosilicates;
2/4	Minerals: Phyllosilicates; Methods: Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM)
2/6	Minerals: Iron and Aluminum Oxides; Method: Mössbauer Spectroscopy
2/11	Minerals: Manganese Oxides, Carbonates;
2/13	Minerals: Sulfides, Sulfates; Water: Structure and Properties; Ions in Solution; Methods: Fourier Transform Infrared (FTIR) Spectroscopy and Raman Spectroscopy
2/18	Structure and Properties of Mineral-Water Interfaces; Surface Charging;
<b>2/20</b>	<b>NO CLASS: Prof. Catalano at NSF Data Management Workshop</b>
2/25	Method: X-ray Reflectivity; Surface Potentials; Surface Complexation Models
2/27	Surface Complexation: Mechanisms and Models
<b>3/3</b>	<b><i>Project 1 Presentations</i></b>
<b>3/5</b>	<b><i>Project 1 Presentations</i></b>
<b>3/10</b>	<b>NO CLASS: Spring Break</b>
<b>3/12</b>	<b>NO CLASS: Spring Break</b>
<b>3/17</b>	<b>NO CLASS: Extended Spring Break</b>
<b>3/19</b>	<b>NO CLASS: Extended Spring Break</b>

- 3/24 Complex Ion Adsorption; Methods: X-ray Absorption Fine Structure (XAFS) Spectroscopy; Mineral Nucleation
- 3/26 Mineral Growth; Methods: Atomic Force Microscopy (AFM) and Scanning Tunneling Microscopy (STM); Silicate Weathering
- 3/31 Silicate Dissolution; Clay Formation
- 4/2 Carbonate Weathering and Precipitation; Dissolution of Oxides and Sulfides
- 4/7 Mineral Surface Redox Reactions; Methods: X-ray Photoelectron Spectroscopy (XPS) and Auger Electron Spectroscopy (AES)
- 4/9 Microbe-Mineral Interactions: Ion Adsorption, Biofilms, Bacterial-Promoted Mineral Dissolution, Microbial Biomineralization; Methods: X-ray Standing Waves (XSW)
- 4/14 Nanominerals: Formation, Stability, and Reactivity; Method: Small Angle X-ray Scattering (SAXS), PDF Analysis of X-ray Scattering Data
- 4/16 Kinetics of Mineral-Water Interface Reactions: Overview, Adsorption, Ostwald Ripening; Computational Methods: Density Functional Theory (DFT) and Molecular Dynamics (MD) Simulations
- 4/21 Kinetics of Mineral-Water Interface Reactions: Nucleation, Crystal Growth, Dissolution; Course Summary
- 4/23 Possible Course Meeting to Accommodate Schedule Changes
- 5/4 Final Papers are due*

**The instructor reserves the right to modify this syllabus during the semester. These changes will be announced in class, and it is the students' responsibility to attend class or make other necessary arrangements to keep abreast of the situation.**