ERTH602 – Theoretical Petrology CRN 88933

Instructor: Julia Hammer (jhammer@hawaii.edu)
Office Hours: by appointment

Meeting times and location: TTh 12:00-1:15 pm POST 708
Credits: 3

Course Learning Objectives. This course prepares students to understand and critically evaluate the theoretical basis for leading quantitative petrologic models involving phase equilibria, through development of fundamental physical chemistry principles and exposure to practical applications of mineral-melt equilibrium models.

Topics include Gibbs free energy and its temperature, pressure, and composition derivatives; phase equilibria and liquid immiscibility; fugacity, activity, and chemical potential; ideal and nonideal solutions; volatile solubilities; kinetic theory; chemical diffusion; and phase transformations.

Teaching and Learning Methods. Lecture is the primary method of material delivery in the classroom. Students will develop a set of notes that will guide them through the essential reading and provide a foundation for practical problem-solving. Applications to igneous petrology, volcanology, and planetary science are emphasized in problem sets and class projects.

Expected Background. This course is intended for graduate students who have an undergraduate-level background in igneous petrology. Math prerequisites are two semesters of college calculus. Linear algebra is helpful. Experience with spreadsheets and MATLAB programming is helpful but not required.

Upon completion of the course, students will be able to

- critically evaluate thermodynamic arguments underpinning published works in the petrological literature
- code petrological models and plot in the MATLAB programming environment

Evaluation

Exam: there will be one mid-term exam that will count 20% toward the course grade. The exam is typically implemented in two stages: an individual portion and a group-work portion. The exam score is a combination of performance on both stages, weighted toward the individual portion. There is no final exam for this course.

Homework: Homework assignments will count 60% toward the course grade. Assignments are generally due a week after they are assigned.

Project: a class project will count 20% toward the course grade and will consist of a written document (including scripts or spreadsheets) and an oral presentation.

Texts. Reading materials will be supplied on our Laulima site as pdf documents. Reading will be assigned from a variety of sources, drawing mainly from Nordstrom and Munoz (1994):
Nordstrom, D.K. and Munoz, J.L., 1994. Geochemical Thermodynamics: Cambridge, Blackwell, 493 p.

Homework problem sets are where we develop skills and intuition. The descriptions below outline the learning goals of each exercise. The problem sets assigned in 2024 may include these and/or other exercises.

HW01. Math and chemistry review: forms of energy; logs and exponents; derivatives and differentials; test a differential for exactness.

HW02. Compare deviations of various gases from ideality by considering critical points, calculating van de Waals constants, plot V-P isotherms, and calculate the compressibility curves that describe the principle of corresponding states. Plot and calculate in Matlab, including loops.

HW03. Work with calorimetric data, and practice integrating the heat capacity polynomial, Cp(T), to understand how enthalpy and entropy changes are computed; use Matlab `polyfit` and `polyval` functions.

HW04. Apply the cyclic relation to examine the adiabatic gradient; use Matlab to compute a phase diagram using thermodynamic data and relationships.
HW05. Work with G-X diagrams in order to understand various binary T-X phase diagram topologies.
HW06. Use the cryoscopic equation to generate a phase diagram and compare the result against the experimentally-determined diagram.
HW07. Explore the Burnham solubility model for H_2O in silicate-melt. Use Matlab to plot results in 3D.
HW08. Calculate fO_2-T buffer curves from thermodynamic data and relationships; determine the mineral mode of a rock using Matlab backslash division; plot mineral compositions in ternary space with Matlab.
HW09. All about olivine: Explore the regular solution model using olivine thermodynamic data and compare the model with the experimentally-determined phase diagram of Bowen and Schairer (1935); examine Fe-Mg exchange equilibrium between olivine and melt and explore compositional/ environmental controls on the exchange coefficient, K_D, by coding the results of Toplis (2005).

Policies and expectations:

• **Assignments**: Homework assignments will be assigned approximately weekly and are due at the beginning of class. The due date will be stated on the assignment. Because it's difficult to ensure uniform grading, late assignments will not be accepted except by pre-arrangement or medical (etc.) emergency.

• **Teamwork**: Students learn best when they work together. Each person is equipped with a different skill set, and you are encouraged to help each other. However, each student must turn in his or her own assignment, composed in his/her own words. A student who fails to follow this rule will receive zero credit for the question, and if the offense is severe, for the assignment.

• **Format**: Neatness, clarity of expression, and completeness are essential to obtain full credit on exams and homework. Helpful tips: (1) Write out the equations, or derive new ones, that you use to solve the problem, and explain (in words) your reasoning. This allows me to allocate partial credit, if the answer is incorrect or the code doesn't run. (2) Show clearly how you solved the problem (e.g., a derivation), including all steps. (4) Check your answer – does your solution make physical sense? Check units.

Explain why you think your answer is correct. If you know it isn't correct, and yet can't figure out why, it's still helpful to explain *how* you know your answer isn't correct.

• **Ethics**. Please adhere to the UH Student Conduct Code at all times (available from the UH Office of Judicial affairs)

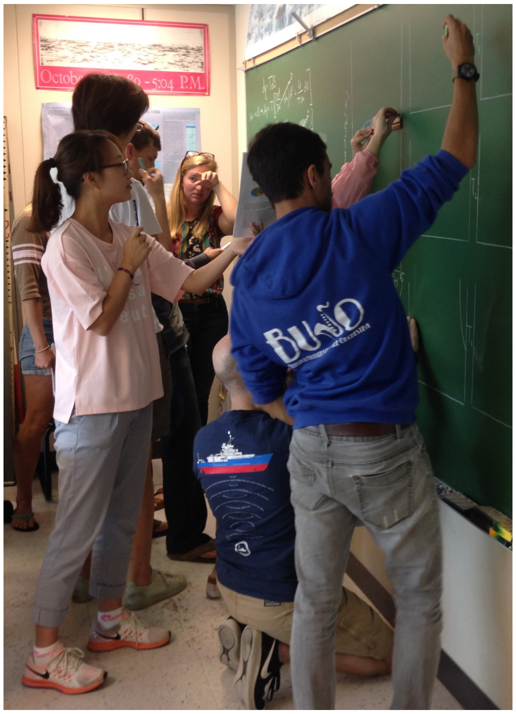
Title IX:

The University of Hawai'i is committed to providing a learning, working and living environment that promotes personal integrity, civility, and mutual respect and is free of all forms of sex discrimination and gender-based violence, including sexual assault, sexual harassment, gender-based harassment, domestic violence, dating violence, and stalking. If you or someone you know is experiencing any of these, the University has staff and resources on your campus to support and assist you. Staff can also direct you to resources that are in the community. Here are some of your options:

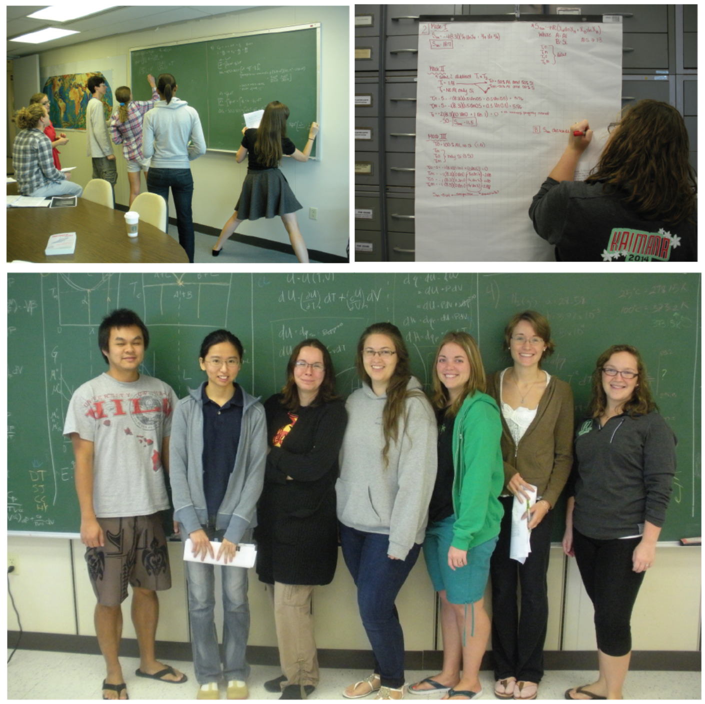
As members of the University faculty, your instructors are required to immediately report any incident of potential sex discrimination or gender-based violence to the campus Title IX Coordinator. Although the Title IX Coordinator and your instructors cannot guarantee confidentiality, you will still have options about how your case will be handled. Our goal is to make sure you are aware of the range of options available to you and have access to the resources and support you need.

If you wish to remain ANONYMOUS, speak with someone CONFIDENTIALLY, or would like to receive information and support in a CONFIDENTIAL setting, use the confidential resources available here: http://www.manoa.hawaii.edu/titleix/resources.html#confidential

If you wish to directly REPORT an incident of sex discrimination or gender-based violence including sexual assault, sexual harassment, gender-based harassment, domestic violence, dating violence or stalking as well as receive information and support, contact: Dee UwonoTitle IX Coordinator (808) 956-2299 t9uhm@hawaii.edu.



Midterm 2017



Midterms 2012 and 2014

Student Feedback from previous offerings

All students of mineralogy, petrology, and geochemistry should take [this course]… It was the only class that helped me learn Matlab, which is really important.

I thought I learned pretty well in my comprehensive exam, but after I took [this] class. I know more principles hide behind the phenomena of reaction and phase transition, like using the Gibbs free energy to predict the conversion rate of our interesting species in this project. Another part impressing me is that the thermodynamic is basic, but it is so powerful. For example, we can calculate the Gibbs free energy of material by measure its heat capacity, in turn, predict the direction of a chemical reaction under high temperature.

I really liked getting the visuals for Gibb's free energy, entropy, enthaply, etc. Pretty confusing at first, but … in the end [they] helped me understand the concepts better.

I am truly glad I took this class, as it … will certainly allow me to read complex thermodynamics better in the literature.