

MSE 401: Thermodynamics of Materials

Fall 2023 Syllabus version July 31, 2023

Homepage <https://canvas.illinois.edu/courses/36947>

3 undergraduate credit hours, 3 graduate credit hours

Credit is not given for both MSE 401 and CHEM 444 or PHYS 427

Lectures are MWF at 9:00-9:50 in Everitt Lab 2310. The lectures will be recorded and made available in Media Space at <https://mediaspace.illinois.edu/channel/MSE+401+2023+Fall/305391132>

Instructor and TAs

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Course Description

Basic thermodynamic principles including energy, entropy, and free energy; macroscopic properties of hard and soft materials systems, such as equilibrium states, phases, and phase transitions. Application of phase diagrams. Statistical interpretation of thermodynamics on the atomistic level.

A theory is the more impressive the greater the simplicity of its premises, the more different kinds of things it relates, and the more extended its area of applicability. Therefore the deep impression that classical thermodynamics made upon me. It is the only physical theory of universal content which I am convinced will never be overthrown, within the framework of applicability of its basic concepts.

-A. Einstein

Lisa, get in here. In this house we obey the laws of thermodynamics!

-Homer Simpson

Course Objectives

Upon completion of the course, students will be able to:

- Define heat and work and explain the concepts of thermodynamic efficiency and reversibility
- State the first and second laws of thermodynamics and describe their significance
- Recognize relationships between thermodynamic state variables and enthalpy, Helmholtz energy, and Gibbs energy.

- Use the laws of thermodynamics to define equilibrium
- Explain the statistical basis for entropy
- Calculate the change in Gibbs energy associated with various processes
- Apply ideal and non-ideal solution models
- Use the thermodynamics of heterogenous mixtures to construct multicomponent phase diagrams
- Evaluate electrochemical reactions

Prerequisites

Credit in MSE 201 or MSE 280

Credit or concurrent registration in MATH 285

Course Expectations and Teaching Philosophy

The focus of this course is on the use of classical thermodynamics for understanding the equilibrium properties of materials. The primary textbook is “Thermodynamics in Materials Science,” second edition, by Robert DeHoff. Professor DeHoff’s text does not emphasize the conceptual framework of thermodynamics. I believe a deeper understanding of the conceptual framework of thermodynamics is a worthwhile intellectual journey. Thus, we will also read an elegant short text by Peter Atkins, “The Laws of Thermodynamics”; and a graphic novel developed by colleagues at Stanford University that takes place in a fantasy world where a team of young scientists are tasked with saving the world without violating the first and second laws.

The design of the course combines lectures, assigned readings, classroom discussion, on-line discussion forums, weekly homework, and assessment by weekly quizzes and a final exam. The homework will include short essay responses to the text, solving problems, calculations, making plots, and drawing diagrams. During lectures, I will sometimes use python in the colab.research.google.com environment to do calculations and illustrate relationships between variables in one-dimensional plots. You will not be required to use computational tools such as python or matlab in the quizzes or exams. You will however be expected to use a science engineering computational tool of your choice in some of the homework problems to do calculations and make plots. We will strive to clearly articulate the assignments, due dates, and grading criteria.

MSE 401 is a 3 credit hour course and therefore requires a time commitment of approximately 9 hours per week. I expect you to spend approximately 3 hours per week attending lectures. You should spend approximately 6 hours per week reviewing lecture material, reading the texts, doing homework, contributing to on-line discussions, and preparing for quizzes and the final exam. I recommend that you schedule a regular time to study.

Web Applications

URL	Purpose
Canvas	Course schedule, homework assignments, gradebook, and posting of text-based resources, e.g., syllabus, homework solutions, and readings in addition to the required texts.
Mediaspace	Posting of recordings of lectures
Campuswire	Discussion form, communications with TAs and Instructor

iClicker	In-class polling
Google Colaboratory	(Optional) Python notebooks

Required Readings

Thermodynamics in Materials Science, second edition, by Robert DeHoff, CRC Press, Taylor and Francis Group, 2006. We will refer to this text as “DeHoff”

The Laws of Thermodynamics: A Very Short Introduction, by Peter Atkins, Oxford University Press, 2010. We will refer to this text as “Atkins”.

The Phoenix Corps, by Petr Johanes, Masami Kiyono, Alberto Salleo, and Colin Reeves-Fortney, copyright Stanford University, 2019. We will refer to this text as “TPC”.

Prof. Salleo kindly made a digital copy of TPC available for use in our course at no charge. You can download a copy for your individual use from our class campuswire.com site. Do not distribute this document electronically or in print to anyone outside of our class.

Course Requirements

1. Use Campuswire class feed and chat rooms for communicating with the instructor, TAs, and peers.
2. Complete assigned readings.
3. Use Canvas to access the course materials and complete assignments within the guidelines established in the course calendar. Submit assignments via Canvas
4. Participate in the in-class polling during lectures.
5. Adhere to assignment deadlines. The deadlines are firm unless a student is given special permission by the instructor. Late submissions are not subject to partial credit.
6. Contact the instructor if special circumstances cause interruption of course activities.

Course Communication

Please contact the instructor or the TAs via the Campuswire discussion forum if you have questions at any time. In person meeting and Zoom or telephone consultations can be arranged outside of regularly scheduled office hours. The instructor and TAs will respond within one business day.

Announcements. The instructor and TAs will use Canvas to make announcements. The default settings of Canvas are that new announcements are also sent immediately by email. You can change that default setting within Canvas if you prefer.

Campuswire. The Campuswire forum is an important part of the course. Please minimize the use of direct messaging and emphasize posting to the entire class. If you want clarification of an assignment or help in understanding the reading, then it is likely that many of your classmates will benefit from your question and will benefit from the responses of classmates, the TAs, or instructor. Feel free to carry on an extended discussion with your classmates independent of feedback from the instructor or TAs. The TAs will intervene if the discussion gets off track.

Netiquette. In any social interaction, certain rules of etiquette are expected and contribute to more enjoyable and productive communication. The following [tips for interacting online](#) are adapted from guidelines originally compiled by Chuq Von Rospach and Gene Spafford at UIS.

- Remember that the person receiving your message is someone like you, someone who deserves and appreciates courtesy and respect.
- Be brief; succinct, thoughtful messages have the greatest impact.
- Your messages reflect on YOU; take time to make sure that you are proud of their form and content.
- Use descriptive subject headings.
- Think about your audience and the relevance of your messages.
- Be careful with humor and sarcasm; without the voice inflections and body language of face-to-face communication, Internet messages can be easily misinterpreted.
- When making follow-up comments, summarize the parts of the message to which you are responding.
- Avoid repeating what has already been said; needless repetition is ineffective communication.
- Cite appropriate references whenever using someone else's ideas, thoughts, or words.

Assessment

Participation (10% of course grade): Participation will be assessed by in-class polling using iClicker. Points will be given for participation in the in-class poll. We will not deduct points for incorrect answers during the in-class polling. We anticipate approximately one poll per class session, i.e., approximately 40 polls during the semester. You will receive full credit for participation if you participate in 70% of the polls administered during the semester.

Homework (30% of course grade): homework is due and submitted electronically in Canvas by 5 pm on the assigned day. Since solutions will be distributed when the homework is due, late submissions will not be accepted. If you have a documented, extenuating circumstance, please communicate with Prof. Cahill for accommodation. The two lowest relative homework scores will be dropped in assigning the 30% of the course grade that comes from homework.

Quizzes (35% of course grade): Quizzes will be administered in person during the first ½ of the class period on Fridays. The two lowest quiz scores will be dropped in assigning the 35% of the course grade that comes from homework. The first quiz will be on Friday September 9.

Comprehensive Final Exam (25% of course grade) during finals week in Everitt 2310: 8-11 AM, Monday December 12.

The overall course grade will be converted to a letter grade on a curved scale. The curved scale will not be harsher than a straight scale (97-100 = A+; 93-97 = A; 90-93 = A-; 87-90 = B+; etc.)

Homework policies

(Acknowledgement of this wording to Prof. Elizabeth Holm at Carnegie Mellon University.)

For the homework sets in this class, you are welcome to work alone or in groups, at your own discretion, so long as the final result is your own.

- You understand and can explain in your own words each step in the solution.
- You independently verified all results and analysis.
- You are personally responsible for the correctness of the answers.
- You gained the knowledge and skills intended from the assignment.

COVID Policy

If you test positive for COVID and are isolating for the 5 day period following the positive test, you are excused participation points, homework due dates, and quizzes during the 5 day isolation period. If you have not fully recovered after the 5 day isolation and unable to attend class, please contact Prof. Cahill.

Academic Integrity Policy

The University of Illinois at Urbana-Champaign Student Code should also be considered as a part of this syllabus. According to the Student Code, "It is the responsibility of each student to refrain from infractions of academic integrity, from conduct that may lead to suspicion of such infractions, and from conduct that aids others in such infractions."

Academic dishonesty may result in a failing grade. Every student is expected to review and abide by the Academic Integrity Policy: <http://studentcode.illinois.edu/>. Ignorance is not an excuse for academic dishonesty. It is your responsibility to read this policy to avoid any misunderstanding. Do not hesitate to ask me if you are ever in doubt about what constitutes plagiarism, cheating, or any other breach of academic integrity.

See also this quick reference guide to academic integrity:

<https://provost.illinois.edu/policies/policies/academic-integrity/students-quick-reference-guide-to-academic-integrity/>

Academic Accommodations

To obtain disability-related academic adjustments and/or auxiliary aids, students with disabilities must contact the course instructor and the Disability Resources and Educational Services (DRES) as soon as possible. To contact DRES, you may visit 1207 S. Oak St., Champaign, call 333-4603 (V/TDD), or e-mail a message to disability@illinois.edu. <http://www.disability.illinois.edu>

Family Educational Rights and Privacy Act

Any student who has suppressed their directory information pursuant to Family Educational Rights and Privacy Act (FERPA) should self-identify to the instructor to ensure protection of the privacy of their attendance in this course. See <https://registrar.illinois.edu/academic-records/ferpa> for more information.

Sexual Misconduct Policy and Reporting

The University of Illinois is committed to combating sexual misconduct. Faculty and staff members are required to report any instances of sexual misconduct to the University's Title IX and Disability Office. In turn, an individual with the Title IX and Disability Office will provide information about rights and options, including accommodations, support services, the campus disciplinary process, and law enforcement options. A list of the designated University employees who, as counselors, confidential advisors, and medical professionals, do not have this reporting responsibility and can maintain confidentiality, can be found at

<https://wecare.illinois.edu/resources/students/#confidential>

Other information about resources and reporting is available at <https://wecare.illinois.edu>

Community of Care

As members of the Illinois community, we each have a responsibility to express care and concern for one another. If you come across a classmate whose behavior concerns you, whether in regards to their well-being or yours, we encourage you to refer this behavior to the Student Assistance Center (217-333-0050 or <http://odos.illinois.edu/community-ofcare/referral/>). Based on your report, the staff in the Student Assistance Center reaches out to students to make sure they have the support they need to be healthy and safe. Further, we understand the impact that struggles with mental health can have on your experience at Illinois. Significant stress, strained relationships, anxiety, excessive worry, alcohol/drug problems, a loss of motivation, or problems with eating and/or sleeping can all interfere with optimal academic performance. We encourage all students to reach out to talk with someone, and we want to make sure you are aware that you can access mental health support at the Counseling Center (<https://counselingcenter.illinois.edu/>) or McKinley Health Center (<https://mckinley.illinois.edu/>). For mental health emergencies, you can call 911 or walk into the Counseling Center, no appointment needed.

Course Schedule

Lecture topics, reading assignments, assignment due dates, and times of quizzes and exams will be posted in Canvas. An overview is given below. The schedule is subject to change.

Week. Topic	Reading
1. The Laws of Thermodynamics	Atkins, Chapters 1-3
2. The Laws of Thermodynamics	Atkins, Chapters 4-5; DeHoff, Chapter 3
3. Thermodynamic Variables and Relations	DeHoff, Chapter 4 .1
4. Thermodynamic Variables and Relations	DeHoff, Chapter 4.2
5. Equilibrium Criteria	DeHoff, Chapter 5
6. Statistical Thermodynamics	TPC, pp-1-37; DeHoff, Chapter 6.1-6.2
7. Statistical Thermodynamics	TPC, pp-38-85; DeHoff, Chapter 6.3
8. One Component Heterogeneous Systems	DeHoff, Chapter 7.1-7.2
9. One Component Heterogeneous Systems	DeHoff, Chapter 7.3-7.5
10. Multicomponent Homogeneous Systems	DeHoff, Chapter 8.1-8.2
11. Multicomponent Homogeneous Systems	DeHoff, Chapter 8.3-8.6
12. Multicomponent Heterogeneous Systems	DeHoff Chapter 9
13. Thermodynamics of Phase Diagrams	DeHoff Chapter 10
14. Chemical Equilibrium and Electrochemistry	DeHoff Chapter 15
15. Electrochemistry	DeHoff Chapter 15