

Molecular Thermodynamics

ECH 6272

Location: FLI 0105

Academic Term: Fall 2023

Class Periods:

Tues: Periods 8-9 | 3:00 – 4:55 pm

Thur: Period 9 | 4:05 - 4:55 pm

Instructor:

Dr. Janani Sampath

jsampath@ufl.edu

321 ChE Building

Office Hours: 10:00 am – 11:00 am Monday and Wednesday

Zoom link for office hours: <https://ufl.zoom.us/j/96760724346>

Supervised Teaching Student:

Please contact through the Canvas website

Nikki Kragt

kragtn@ufl.edu

Office hours: 10:30 am – 12:30 pm Thursday

Zoom link for office hours: xxx

Course Description

This course will provide a rigorous, microscopic framework to understand classical thermodynamics, this framework is known by many names, we will refer to it as statistical mechanics. In its purest form, thermodynamics only concerns macroscopic properties, like temperature, pressure, volume. It does not care that matter is made up of atoms and molecules. On the other hand, statistical mechanics seeks to compute macroscopic properties from a microscopic model, and in this way understand the different molecular driving forces give rise to various thermodynamic phenomena and laws.

Course Pre-Requisites / Co-Requisites

{basic knowledge is sufficient; we will review these at the beginning of the term}

Undergraduate chemical engineering thermodynamics

Multivariate integral and differential calculus

Basic statistics and probability

Recommended Textbooks and Software

Introduction to Modern Statistical Mechanics

David Chandler

Molecular Driving Forces

Ken Dill and Sarina Bromberg

Thermodynamics and Statistical Mechanics: An Integrated Approach

Scott Shell

Exams and Quizzes:

There will be 2 exams during the semester. **The final exam will be on December 12th.** There will be 2 announced quizzes during the semester. Quizzes will be announced at least 1 week in advance. No credit will be given for problems that have a solution but all the work leading to this solution is not shown. Partial credit will be assigned based on the rules that will be consistently applied to all students.

All quizzes and exams are open note/open book, but not open internet. On the day of the exam, we will have a review class.

Homework:

- You will have a total of 5 homework sets.
- Solutions will be posted on the course website.
- The homework must be turned in on canvas by the due date.
- Late homework will be accepted only with instructor approval. As a rule, there will be a 20% penalty for each day it is late. No late homework accepted after the solutions are posted.
- No credit will be given for problems that only have a solution without the work leading to the solution.

Tentative Course Schedule

Weeks 1,2: Multivariate calculus and probability, Macroscopic thermodynamics (heat, work, first and second laws)

Weeks 3,4: Entropy and combinatorics, Entropy and equilibrium

Weeks 5,6: Molecular view of energy | **Exam 1**

Weeks 7,8: Statistical mechanics and ensembles

Weeks 9,10: Ideal gas (mono- di- and poly-atomic) and kinetic theory of gases

Weeks 11,12: Importance of fluctuations, statistical mechanics of interfaces, and mixtures | **Exam 2**

Weeks 13,14: Statistical Mechanics of Phase Transitions, Ideal quantum gases

Weeks 15: Transition state theory, Monte Carlo and Molecular Dynamics Simulations | **Final**

Online Course Recording

Our class sessions may be audio visually recorded for students in the class to refer back and for enrolled students who are unable to attend live. Students who participate with their camera engaged or utilize a profile image are agreeing to have their video or image recorded. If you are unwilling to consent to have your profile or video image recorded, be sure to keep your camera off and do not use a profile image. Likewise, students who un-mute during class and participate orally are agreeing to have their voices recorded. If you are not willing to consent to have your voice recorded during class, you will need to keep your mute button activated and communicate exclusively using the "chat" feature, which allows students to type questions and comments live. The chat will not be recorded or shared. As in all courses, unauthorized recording and unauthorized sharing of recorded materials is prohibited.

Attendance Policy, Class Expectations, and Make-Up Policy:

Class attendance is strongly recommended. If you are unwell, inform the instructor in advance. Requests for make-up tests will be granted only if appropriate documentation about illness, family emergency or UF-related travel are given to the instructor.

Evaluation of Grades:

Assignment	Total Points	Percentage of Final Grade
Homework Sets (7)	10 each	15%
Quizzes (2)	10 each	15%
Midterm Exam 1, 09/28	100	20%
Midterm Exam 2, 10/31	100	20%
Final Exam, 12/15	100	30%

Grading Policy:

Final grades will be assigned using the standard deviation (σ) method. The scale for the course will be as follows:

Percent	Grade	Grade Points
Mean + σ < Score	A	4.00
Mean + 0.67 σ < Score \leq Mean + σ	A-	3.67
Mean + 0.33 σ < Score \leq Mean + 0.67 σ	B+	3.33
Mean < Score \leq Mean + 0.33 σ	B	3.00
Mean - 0.33 σ < Score \leq Mean	B-	2.67
Mean - 0.67 σ < Score \leq Mean - 0.33 σ	C+	2.33
Mean - σ < Score \leq Mean - 0.67 σ	C	2.00
Mean - 1.33 σ < Score \leq Mean - σ	C-	1.67
Mean - 1.67 σ < Score \leq Mean - 1.33 σ	D+	1.33
Mean - 2 σ < Score \leq Mean - 1.67 σ	D	1.00
Mean - 2.33 σ < Score \leq Mean - 2 σ	D-	0.67
Score \leq Mean - 2.33 σ	E	0.00

Instructor may lower the threshold for attaining the letter grades specified above (to the benefit of the students), but will not raise the threshold.

More information on UF grading policy may be found at:

<https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx>

Students Requiring Accommodations:

Students with disabilities who experience learning barriers and would like to request academic accommodations should connect with the disability Resource Center by visiting <https://disability.ufl.edu/students/get-started/>. It is important for students to share their accommodation letter with their instructor and discuss their access needs, as early as possible in the semester.

Course Evaluation:

Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available at <https://gatorevals.aa.ufl.edu/students/>. Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their Canvas course menu under GatorEvals, or via <https://ufl.bluera.com/ufl/>. Summaries of course evaluation results are available to students at <https://gatorevals.aa.ufl.edu/public-results/>.

University Honesty Policy:

UF students are bound by The Honor Pledge which states, "We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honor and integrity by abiding by the Honor Code. On all work submitted for credit by students at the University of Florida, the following pledge is either required or implied: "On my honor, I have neither given nor received unauthorized aid in doing this assignment." The Honor Code (<https://sccr.dso.ufl.edu/policies/student-honor-code-student-conduct-code/>) specifies a number of behaviors that are in violation of this code and the possible sanctions. Furthermore, you are obligated to report any condition that facilitates academic misconduct to appropriate personnel. If you have any questions or concerns, please consult with the instructor or TAs in this class.

Commitment to a Safe and Inclusive Learning Environment:

The Herbert Wertheim College of Engineering values broad diversity within our community and is committed to individual and group empowerment, inclusion, and the elimination of discrimination. It is expected that every person in this class will treat one another with dignity and respect regardless of gender, sexuality, disability, age, socioeconomic status, ethnicity, race, and culture.

If you feel like your performance in class is being impacted by discrimination or harassment of any kind, please contact your instructor or any of the following:

- Your academic advisor or Graduate Program Coordinator
- Robin Bielling, Director of Human Resources, 352-392-0903, rbielling@eng.ufl.edu
- Curtis Taylor, Associate Dean of Student Affairs, 352-392-2177, taylor@eng.ufl.edu
- Toshikazu Nishida, Associate Dean of Academic Affairs, 352-392-0943, nishida@eng.ufl.edu

Software Use:

All faculty, staff, and students of the University are required and expected to obey the laws and legal agreements governing software use. Failure to do so can lead to monetary damages and/or criminal penalties for the individual violator. Because such violations are also against University policies and rules, disciplinary action will be taken as appropriate. We, the members of the University of Florida community, pledge to uphold ourselves and our peers to the highest standards of honesty and integrity.

Student Privacy:

There are federal laws protecting your privacy with regards to grades earned in courses and on individual assignments. For more information, please see: <https://registrar.ufl.edu/ferpa.html>

Campus Resources:

Health and Wellness

U Matter, We Care:

Your well-being is important to the University of Florida. The U Matter, We Care initiative is committed to creating a culture of care on our campus by encouraging members of our community to look out for one another and to reach out for help if a member of our community is in need. If you or a friend is in distress, please contact umatter@ufl.edu so that the U Matter, We Care Team can reach out to the student in distress. A nighttime and weekend crisis counselor is available by phone at 352-392-1575. The U Matter, We Care Team can help connect students to the many other helping resources available including, but not limited to, Victim Advocates, Housing staff, and the Counseling and Wellness Center. Please remember that asking for help is a sign of strength. In case of emergency, call 9-1-1.

Counseling and Wellness Center: <http://www.counseling.ufl.edu/cwc>, and 392-1575; and the University Police Department: 392-1111 or 9-1-1 for emergencies.

Sexual Discrimination, Harassment, Assault, or Violence

If you or a friend has been subjected to sexual discrimination, sexual harassment, sexual assault, or violence contact the [Office of Title IX Compliance](mailto:title-ix@ufl.edu), located at Yon Hall Room 427, 1908 Stadium Road, (352) 273-1094, title-ix@ufl.edu

Sexual Assault Recovery Services (SARS)

Student Health Care Center, 392-1161.

University Police Department at 392-1111 (or 9-1-1 for emergencies), or <http://www.police.ufl.edu/>.

Academic Resources

E-learning technical support, 352-392-4357 (select option 2) or e-mail to Learning-support@ufl.edu.
<https://lss.at.ufl.edu/help.shtml>.

Career Resource Center, Reitz Union, 392-1601. Career assistance and counseling. <https://www.crc.ufl.edu/>.

Library Support, <http://cms.uflib.ufl.edu/ask>. Various ways to receive assistance with respect to using the libraries or finding resources.

Teaching Center, Broward Hall, 392-2010 or 392-6420. General study skills and tutoring.
<https://teachingcenter.ufl.edu/>.

Writing Studio, 302 Tigert Hall, 846-1138. Help brainstorming, formatting, and writing papers.
<https://writing.ufl.edu/writing-studio/>.

Student Complaints Campus: <https://care.dso.ufl.edu>.

On-Line Students Complaints: <http://www.distance.ufl.edu/student-complaint-process>.