

Biomolecular Thermodynamics and Kinetics

BME 4621 Section 20216

Class Periods: M W F, 6th Period, 12:50-1:40 PM

Location: Larsen 310

Academic Term: Fall 2024

Instructor:

Gregory A. Hudalla

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352-273-9326

Office Hours: Monday 2-3PM & Friday 11:30-12:30PM

Teaching Assistant/Peer Mentor/Supervised Teaching Student:

Please contact through the Canvas website

- Cameron Manson, cameronmanson@ufl.edu

Course Description

Principles of thermodynamics and kinetics from a biomolecular perspective. The mathematics, analysis, and applications of classical thermodynamics, statistical thermodynamics, and reaction kinetics will be introduced in the context of molecular interactions, binding equilibria, metabolism, and biomolecular transport common to living systems.

Course Pre-Requisites / Co-Requisites

BME 3060, BME 4311

Course Objectives

- Develop basic knowledge of classical thermodynamics, equilibrium, and reaction kinetics.
- Develop an understanding of the application of statistical thermodynamics to biomolecule behavior and interactions.
- Develop a competence in the fundamental analytical and computational tools used to describe energy transformation within living systems.

Materials and Supply Fees

None

Relation to Program Outcomes (ABET):

| Outcome | Coverage* |
|---|------------------|
| 1. An ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics | High, emphasized |
| 2. An ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors | |
| 3. An ability to communicate effectively with a range of audiences | |
| 4. An ability to recognize ethical and professional responsibilities in engineering situations and make informed judgments, which must consider the impact of engineering solutions in global, economic, environmental, and societal contexts | |

| | |
|---|--------|
| 5. An ability to function effectively on a team whose members together provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives | |
| 6. An ability to develop and conduct appropriate experimentation, analyze and interpret data, and use engineering judgment to draw conclusions | |
| 7. An ability to acquire and apply new knowledge as needed, using appropriate learning strategies | Medium |

Required Textbooks and Software

Title: Biomolecular Thermodynamics: From Theory to Application

Author: Barrick, Douglas

Publication date and Edition: 2017, 1st edition; CRC Press

ISBN: 978-1-4398-0019-5

Recommended Materials

Title: *Biological Thermodynamics*

Author: Haynie, Donald T.

Publication date and edition: 2008, 2rd edition; Cambridge

ISBN number: 978-0-5217-1134-0

Title: *Molecular Driving Forces: Statistical Thermodynamics in Chemistry and Biology.*

Author: Dill, Ken A., and Bromberg, S.

Publication date: 2002, Routledge

ISBN: 978-0-8153-2051-7.

Title: *Biochemical Engineering Fundamentals*

Author: Bailey, James E., and Ollis, David F.

Publication date: 1986, 2rd edition, McGraw-Hill

ISBN: 978-0-0706-6601-6

Course Schedule

| Week | Topic |
|---------------|---|
| <u>PART 1</u> | |
| 1 | Overview of energy transformation in living systems |
| 2 | First law of thermodynamics – Barrick 3 |
| 3 | Second law of thermodynamics – Barrick 4 |
| 4 | Gibbs Free Energy – Theory I – Barrick 5 |
| 5 | Gibbs Free Energy – Theory II |
| 6 | Gibbs Free Energy – Applications I |
| 7 | Gibbs Free Energy – Applications II |
| <u>PART 2</u> | |
| 8 | Statistical Thermodynamics - Theory – Barrick 8, 9 |
| 9 | Statistical Thermodynamics - Application |
| 10 | Binding Equilibria – Barrick 13, 14 |
| 11 | Cooperativity/Allostery |
| 12 | Reaction kinetics - Theory |
| 13 | Reaction kinetics – Modeling I |
| 14 | Reaction kinetics – Modeling II |
| 15 | Biology, complexity, and evolution |

Assessment dates:

Problem sets (due Fridays by midnight via Canvas unless noted): Sept 6 (set 1 and 2), Sept 20, Sept 27, Oct 11, Oct 18, Nov 1, Nov 8, Nov 22 (set 9 and 10)

Quizzes: Sept 13, Oct 4, Oct 25, Nov 15, Dec 4

Attendance Policy, Class Expectations, and Make-Up Policy

-Attendance is not mandatory and will not be recorded. Announcements will be delivered via Canvas.

-Problem sets are to be submitted via Canvas on the day that they are due.

-You must let me know AS SOON AS POSSIBLE if you will be ABSENT on the SCHEDULED DATE of ANY quiz. If you know that you'll be absent for a QUIZ, a make-up **MUST** be taken **PRIOR TO** the date listed above. **No make-up quizzes or exams will be given for unexcused absences.** Excused absences are consistent with university policies in the undergraduate catalog (<https://catalog.ufl.edu/ugrad/current/regulations/info/attendance.aspx>) and require appropriate documentation.

<https://catalog.ufl.edu/UGRD/academic-regulations/attendance-policies/>

Evaluation of Grades

| Assignment | Total Points | Percentage of Final Grade |
|-------------------|---------------|---------------------------|
| Problem Sets (10) | 100 | 33.3% |
| Quizzes (5) | 200 (40 each) | 66.7% |
| Total | 300 | 100% |

Grading Policy

| Percent | Grade | Grade Points |
|--------------|-------|--------------|
| 94 - 100 | A | 4.00 |
| 90.0 - 93.99 | A- | 3.67 |
| 87 - 89.99 | B+ | 3.33 |
| 83 - 86.99 | B | 3.00 |
| 80 - 82.99 | B- | 2.67 |
| 77 - 79.99 | C+ | 2.33 |
| 73- 76.99 | C | 2.00 |
| 70 - 72.99 | C- | 1.67 |
| 67 - 69.99 | D+ | 1.33 |
| 63 - 66.99 | D | 1.00 |
| 60 - 62.99 | D- | 0.67 |
| 0 - 59.99 | E | 0.00 |

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.ua.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.ua.ufl.edu/public-results/>.

In-Class Recording

Students are allowed to record video or audio of class lectures. However, the purposes for which these recordings may be used are strictly controlled. The only allowable purposes are (1) for personal educational use, (2) in connection with a complaint to the university, or (3) as evidence in, or in preparation for, a criminal or civil proceeding. All other purposes are prohibited. Specifically, students may not publish recorded lectures without the written consent of the instructor.

A “class lecture” is an educational presentation intended to inform or teach enrolled students about a particular subject, including any instructor-led discussions that form part of the presentation, and delivered by any instructor hired or appointed by the University, or by a guest instructor, as part of a University of Florida course. A class lecture does not include lab sessions, student presentations, clinical presentations such as patient history, academic exercises involving solely student participation, assessments (quizzes, tests, exams), field trips, private conversations between students in the class or between a student and the faculty or lecturer during a class session.

Publication without permission of the instructor is prohibited. To “publish” means to share, transmit, circulate, distribute, or provide access to a recording, regardless of format or medium, to another person (or persons), including but not limited to another student within the same class section. Additionally, a recording, or transcript of a recording, is considered published if it is posted on or uploaded to, in whole or in part, any media platform, including but not limited to social media, book, magazine, newspaper, leaflet, or third party note/tutoring services.

A student who publishes a recording without written consent may be subject to a civil cause of action instituted by a person injured by the publication and/or discipline under UF Regulation 4.040 Student Honor Code and Student Conduct Code.

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/process/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 varied perspectives and lived experiences within our community and is committed to supporting the University's core values, including the elimination of discrimination. It is expected that every person in this class will treat one another with dignity and respect regardless of race, creed, color, religion, age, disability, sex, sexual orientation, gender identity and expression, marital status, national origin, political opinions or affiliations, genetic information, and veteran status.

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 Undergraduate Coordinator
- HWCOE Human Resources, 352-392-0904, student-support-hr@eng.ufl.edu
- Pam Dickrell, Associate Dean of Student Affairs, 352-392-2177, pld@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: <https://counseling.ufl.edu>, 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**, 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://elearning.ufl.edu/>.

Career Connections Center, Reitz Union, 392-1601. Career assistance and counseling; <https://career.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://sccr.dso.ufl.edu/policies/student-honor-code-student-conduct-code/>; <https://care.dso.ufl.edu>.

On-Line Students Complaints: <https://distance.ufl.edu/getting-help/>; <https://distance.ufl.edu/state-authorization-status/#student-complaint>.