

## AI for Materials

EMA 4935

**Class Periods:** Days Tuesday, Periods 8-9 (3:00 PM - 4:55 PM), Thursday, Period 9 (4:05 PM - 4:55 PM)

**Location:** NEB 100

**Academic Term:** Spring 2024

### Instructors:

Prof. Richard G. Hennig

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Office Hours: TBA

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### Teaching Assistant/Peer Mentor/Supervised Teaching Student:

Please contact through the Canvas website

□ TBA

### Course Description

Special Topics in Materials Science and Engineering

### Course Pre-Requisites / Co-Requisites

No prerequisite. Knowledge of vector and matrix algebra, derivatives and integrals, probabilities and random variables statistics, and some experience in coding in any language, such as Python (preferred), MATLAB, Java, C.

### Course Objectives

In this course, you will review the mathematical fundamentals of data science and machine learning, gain hands-on experience developing software using Python and data science tools, and apply AI techniques to materials data, structures, and processes to develop the skills needed to address real-world engineering problems.

### Required Textbooks and Software

- *Machine Learning in Materials Science* by Keith T. Butler, Felipe Oviedo, Pieremanuele Canepa
- Freely available at <https://doi.org/10.1021/acsinfocus.7e5033>

### Course Schedule

Week	Class Dates	Topic	Book Chapter
1	January 9 January 11	Introduction Programming Tools: Introduction to Python	
2	January 16 January 18	Math Review Probability and Statistics Linear Algebra and Differential Calculus	
3	January 23 January 25	Data Science Tools: Materials Databases and Pandas Data Frames Univariate and Multivariate Linear Regression	
4	January 30 February 1	1. Applying Machine Learning (ML) to Materials Science Data and Databases Representations and Representation Learning & Evaluation	1
5	February 6 February 8	2. Building Trust in Machine Learning Convolutional Neural Networks (CNNs)	2
6	February 13 February 15	Advanced Validation Uncertainty Quantification and Interpretability	2
7	February 20 February 22	3. Machine Learning for Materials Simulations Representing Materials for ML	3
8	February 27 February 29	Which Representation Is Best? Ultra-fast Force Fields	3
9	March 5	4. Analyzing Experimental Data	4

	March 7	Machine Learning for Electron Microscopy (EM)	
Spring Break			
10	March 19 March 21	Machine Learning for Diffraction ML Analysis of Spectral Data	4
12	March 26 March 28	5. Closed-Loop Optimization and Active Learning for Materials Black-Box Optimization	5
13	April 2 April 4	Bayesian Optimization Including Domain Knowledge into Black-Box Optimization	5
14	April 9 April 11	Navigating High-Dimensional Spaces Bayesian Implementations and Other Efficient Algorithms	5
15	April 16 April 18	6. Discovering New Materials High-Throughput Virtual Screening Direct Optimization with Generative Models	6
16	April 23	Multiobjective Optimization	6

### ***Attendance Policy, Class Expectations, and Make-Up Policy***

#### **Course Website**

The course website is on the Canvas system <https://ufl.instructure.com>, where you can find the announcements, syllabus, pre-recorded video lectures, lecture notes, and homework assignments. We will also use Canvas for the preparatory quizzes, the course exams, and your grades. Please check it frequently.

#### **Flipped Classroom**

The course will utilize a flipped classroom model. A flipped classroom is a teaching approach where you will first explore new content outside the class by viewing a **pre-recorded video lecture** and completing a **preparatory quiz** on Canvas.

Our regularly scheduled online class time is organized around student engagement, inquiry, and assessment, allowing us to elaborate on thermodynamic concepts and apply them to material problems. The in-class sessions will typically entail structured discussions, collaborative problem-solving, and case studies. The in-class session will also be recorded and posted on Canvas.

Flipped classrooms improved the student performance and learning experience effectively (see, for example <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6852382/>). To take advantage of the in-class discussion and problem-solving requires everyone to watch the video lecture before the in-class activity and complete the quiz. Active participation and engagement in class will help you understand the material and acquire the skills to utilize thermodynamics to solve material problems you will encounter throughout your career. I expect attendance. Questions are highly encouraged. If you do not understand something, chances are that your classmates have missed that point, too. You are responsible for material presented in lectures, reading assignments, homework, and distributed notes.

#### **Homework**

Three homework exercises will be assigned. These homework questions are essential to your study and prepare you for the exams. Some exam questions will be adapted from homework. Homework is usually due back seven days before the corresponding exam. The submission dates will be posted in the e-learning assignments. The purpose of homework is to give you an opportunity to evaluate and apply your knowledge. You may collaborate on homework; however, the submitted assignment must represent your own work and preparation. Please ask during the online class to discuss homework problems.

**Homework in its entirety must be word-processed.** For some problems, you will require a suitable math package with graphing capability, e.g., Excel, MatLab, Python. Files have to be pdf, doc, docx, or pptx. Picture files (jpg, etc.) are not accepted.

Homework needs to be submitted online on e-learning. Email is not acceptable for submission of homework. Hard copies are also not accepted.

Homework will be evaluated on the following basis:

	100	85	70	0
<b>Completion</b>	All assigned work is complete.	Most assigned work is complete.	Some assigned work is complete.	Assignment not complete.
<b>Accuracy</b>	All answers are correct.	Most answers are correct.	Some answers are correct.	Little to no answers are correct.
<b>Work shown (derivations and figures)</b>	All work shown in detail.	Most work shown in detail.	Several steps or figures missing.	Did not show any work.

No credit will be given for late unexcused submissions.

### Quizzes and Interactive Learning

We will have online preparatory quizzes covering current and recent lecture material. The quizzes will typically consist of ten questions that should take about 20 minutes to answer. The quizzes serve as feedback both for you and me that you understood the pre-recorded video lectures.

### Exams

We will have three Canvas exams. The exams will consist of concept questions to evaluate your familiarity with the course content and numerical problems designed to test your ability to apply concepts to new situations, i.e., to promote critical thinking. Unless otherwise informed, one sheet of prepared personal notes may be used to assist you in completing examinations. The exams will be on Canvas and use HonorLock. Exam work must be individual, and collaboration is never allowed. Observations of cheating will be promptly reported by the exam proctor. Please see UF's statement on academic honesty: <https://www.dso.ufl.edu/%20sccr/process/student-conduct-honor-code>.

There is no final exam in this class. Exam dates are tentatively scheduled for:

Exam 1: January

Exam 2: March

Exam 3: April

### Exam Conflicts with other course exams

The official UF policy on exam conflict resolution states that when two exams conflict, the course with the higher number will take priority.

### Make-up exams

Make up exams will be provided only with the **prior approval of the instructor**. Excused absences must be consistent with university policies in the Graduate Catalog (<https://catalog.ufl.edu/graduate/regulations>) and require appropriate documentation. Additional information can be found here: <https://catalog.ufl.edu/UGRD/academic-regulations/attendance-policies/>. In general, acceptable reasons for excused absence from an exam include illness, serious family emergencies, special curricular requirements, military obligation, court-imposed legal obligations, and religious holidays. In all cases, you will be required to provide written documentation, and obtain prior instructor approval. You will not be excused from any exam without following the policy above, with no exceptions. Students not in attendance for the scheduled exam will receive a score of zero. **You must notify the instructor no less than 1 week of the scheduled exam of your intent and justification for missing the exam.** Make-up exams for excused absences as well as exam conflicts must occur within 1 week of the missed exam and may occur before the missed exam.

### Grading Policy

Course Title, Prefix, and Number

Course Instructor and Academic Term

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Assignment	Total Points	Percentage of Final Grade
Homework Sets (3)	100 each	20%
Quizzes (about 10)	varies	20%
Midterm Exams (3)	100 each	60%
		100%

Percent	Grade	Grade Points
93.4 - 100	A	4.00
90.0 - 93.3	A-	3.67
86.7 - 89.9	B+	3.33
83.4 - 86.6	B	3.00
80.0 - 83.3	B-	2.67
76.7 - 79.9	C+	2.33
73.4 - 76.6	C	2.00
70.0 - 73.3	C-	1.67
66.7 - 69.9	D+	1.33
63.4 - 66.6	D	1.00
60.0 - 63.3	D-	0.67
0 - 59.9	E	0.00

More information on UF grading policy may be found at:

[UF Graduate Catalog](#)  
[Grades and Grading Policies](#)

### ***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/>.

### ***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 Graduate Program Coordinator
- HWCoe Human Resources, 352-392-0904, [student-support-hr@eng.ufl.edu](mailto:student-support-hr@eng.ufl.edu)
- Curtis Taylor, Associate Dean of Student Affairs, 352-392-2177, [taylor@eng.ufl.edu](mailto:taylor@eng.ufl.edu)
- Toshikazu Nishida, Associate Dean of Academic Affairs, 352-392-0943, [nishida@eng.ufl.edu](mailto: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 regard 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](mailto: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](mailto: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 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>.