Welcome to
CHE 384T: Computational Methods in Materials Science

Introduction to Computational Materials Science

LeSar Ch. 1, App. A

The University of Texas at Austin
McKetta Department
of Chemical Engineering
Cockrell School of Engineering

Lecture Outline

About the course: lecture topics, peer review grading scheme, class policies, etc.

What is Computational Materials Science?

- What is Materials Science?
- What is computation and simulation?

Length and time scales

Developing a model

Examples of computation and simulation in materials science

About this course

This course is an introductory survey to simulation techniques used in materials science for modeling materials phenomena. Materials science is about understanding and predicting how (solid-state) materials respond to various stimuli (e.g., thermal, chemical, mechanical, optical, electrical), and using that understanding to engineer better materials.

The emphasis of this course is on developing a mathematical, algorithmic, and physical understanding for materials simulation. The methods covered in this course will be connected to several on-going research areas and technological applications in chemical engineering and materials science.

Learning objectives

By the end of this course, students will be expected to be able to:

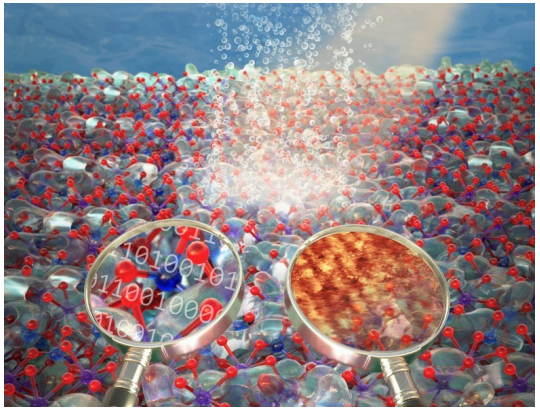
- **Implement** materials modeling methods using basic principles and concepts of scientific coding
- **Generate**, analyze, and visualize simulated data
- **Interpret** simulate data and explain its physical significance
- **Propose** physical models for modeling complex materials phenomena, identify their assumptions and limitations, and suggest improvements to the simulation
- **Communicate** (oral and written) their results to a general audience

About this course

CLASS TIMES: 09:00 am – 10:00 am on Mondays, Wednesdays, and Fridays in CPE 2.222

Instructor: Wennie Wang

Office: CPE 4.450
Office hours: by appointment
Email:wwwennie@che.utexas.edu
Phone: 512-471-9894
Pronouns: she/her/hers



About the instructor:

Education

- Postdoc, Molecular Engineering, UChicago
- Ph.D. Materials, UC Santa Barbara
- B.S. Materials Science & Engineering, MIT

Research (https://wangmaterialsgroup.com)

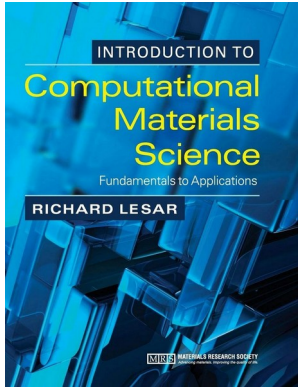
Computational Engineering of optoelectronic materials for sustainability

- Photoelectrochemical properties for clean/value-added fuels
- Neuromorphic computing for energy-efficient computing

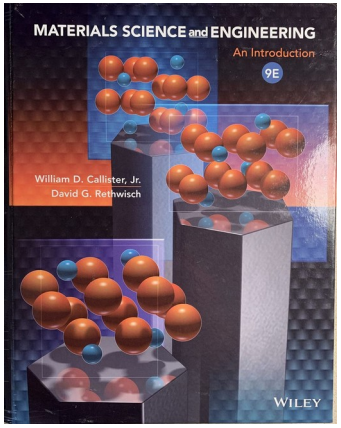
About this course

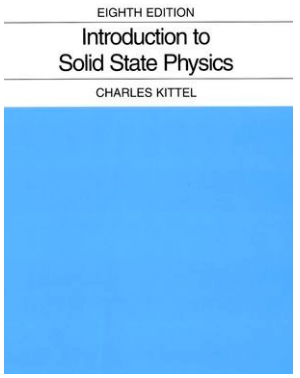
Things you want to have access to:

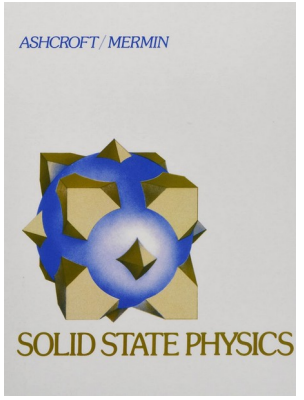
- LeSar → main text
- A computer/work station



Other helpful texts







Course webite: Canvas, https://utexas.instructure.com/courses/1400861

- Assignments
- Files

This course will be taught in Python.
If you prefer another programming language, please inform the instructor

Class Topic	Reading (LeSar)	Notes
Introduction to materials modeling and simulation	Ch. 1, Appendix A	
A brief introduction to crystallography	Appendix B1-B5	
Random Walk Diffusion	Ch. 2, Appendix B7, C5, I2-I3	PS1, see also Ch. 8
Simulation of finite systems	Ch. 3	PS2
Interatomic potentials	Ch. 5, Appendix D4	PS3
Molecular dynamics	Ch. 6, Appendix I4	PS4
Molecular dynamics and connection to stat mech	Appendix G	
Monte Carlo	Ch. 7, Appendix C4, D1-D4	PS5
Kinetic Monte Carlo	Ch. 9	
Monte Carlo at the mesoscale	Ch. 10	
Cellular Automata^	Ch. 11	
Electronic Structure methods^	Ch. 4, Appendix F	
Machine learning in materials science^	Ch. 14	

Approximate readings on Canvas

Lectures will be recorded and made available as announced through Lecture Online

Blank lecture notes posted before class

Annotated notes posted a few days after class

About this course

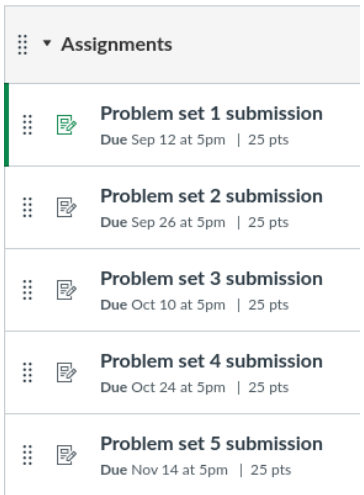
GRADES

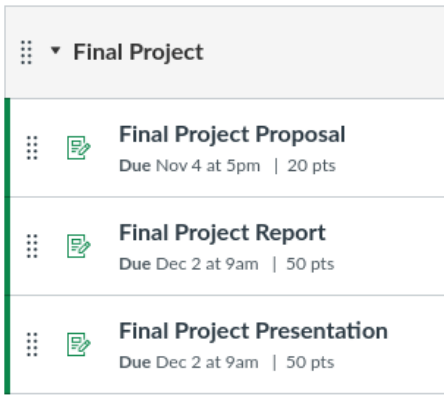
Coursework Breakdown:

- Homework (50%): upload to Canvas by the deadline indicated. **Late work:** This course will have a relatively heavy component of peer review. As such, it is highly recommended to submit by the deadline. If you anticipate a submission delay or require an extension, please arrange ahead of time with the instructor.
- Peer participation (25%): surveys, class discussion, in-class activities
- Final Project (5% proposal, 10% report, 10% presentation): upload to Canvas by the deadlines indicated

Grade breakdown:

> 90% (A), 88-89% (A-), 82-87% (B+), 75-82% (B), 71-75% (B-), 68-71% (C+), 58-68% (C), 55-58% (C-), 50-55% (D), < 50% (F)





First deadline is listed on Canvas

Re-submission (with improvements) is 1 week later

Peer review and scheduling

https://utexas.instructure.com/courses/1400861/files/?preview=79032217

Programming Days (approximately every other Friday):

1	F Aug 30	Installation/set up; Jupyter, Modules and packages, environments What is object oriented programming? Why Python?
2	F Sep 6	Hello World, variable types, global v local variables, manipulating lists and arrays, operators, (formatting strings), sets, tuples, lists, dictionaries, dataframes
3	F Sep 20	conditions, loops, functions, classes and objects
4	F Oct 4	opening a github account, testbeds, measuring speed and optimizing code, C libraries
5	F Oct 18	Peer sharing of Python tricks
6	F Nov 1	Python extras: list comprehension, exception handling decorators, lambda functions, regular expressions

Programming Days are crash courses in programming and help with code implementation

Remaining Fridays are peer review of reports and project proposal

About this course

USE OF CHATGPT

The use of ChatGPT is permitted but any work submitted must reflect the effort and understanding of the student. To get the most out of the course, students are encouraged to take the time to understand and critically evaluate the output. ChatGPT is a generative language learning model. As such, ChatGPT is not always capable of producing reliable or truthful statements. Nevertheless, it can provide a useful starting point when prompted appropriately.

For additional guidelines and ideas, see e.g., Buriak et al. "Best Practices for Using AI When Writing Scientific Manuscripts." *ACS Nano* editorial. Feb 27, 2023. https://pubs.acs.org/doi/10.1021/acsnano.3c01544

ACADEMIC INTEGRITY EXPECTATIONS

You are expected to uphold all standards of academic integrity described in the University Code of Conduct and the Student Honor Code.

About this course

Due 08/26, 11:59 pm

Self introductions

Due 08/30, 11:59pm

Python Pre-test

About this course

OFFICE HOURS

Office hours are open-door policy, meaning you are welcome to discuss topics including and beyond the course material (e.g., career advice, doing research). Please come by!
We will do either completely in-person office hours or completely remote office hours, as announced on Canvas.

SERVICES FOR STUDENTS WITH DISABILITIES (SSD)

I am committed to creating an accessible and inclusive learning environment in this class. Please let me know if you experience any barriers to learning so I can work with you to ensure you have equal opportunity to participate fully in this course. If you are a student with a disability, or think you may have a disability, and need accommodations please contact Services for Students with Disabilities (SSD). Please refer to SSD's website for contact and more information: http://diversity.utexas.edu/disability/.

If you are already registered with SSD, please discuss with and/or deliver your Accommodation Letter to Prof. Wang at the start of the semester your accommodations and needs in this course.

COUNSELING AND MENTAL HEALTH CENTER (CMHC)

If you or anyone you know is experiencing symptoms of stress, anxiety, depression, academic concerns, loneliness, difficulty sleeping, or any other concern impacting your wellbeing – you are strongly encouraged to connect with CMHC. The Counseling and Mental Health Center provides a wide variety of mental health services to all UT students including crisis services, counseling services with immediate support and well-being resources. Additionally, CARE Counselors are located within the academic schools and colleges. These counselors get to know the concerns that are unique to their college's students. For more information on CMHC, visit https://cmhc.utexas.edu or call 512-471-3515.

TITLE IX DISCLOSURE

Beginning January 1, 2020, TexasSenate Bill 212 requires all employees of Texas universities, including faculty, to report any information to theTitle IX Office regarding sexual harassment, sexual assault, dating violence and stalking that is disclosed to them. Texas law requires that all employees who witness or receive any information of this type (including, but not limited to, writing assignments, class discussions, or one-on-one conversations) must be reported. If you would like to speak with someone who can provide support or remedies without making an official report to the university, please email advocate@austin.utexas.edu. For more information about reporting options and resources, visit http://www.titleix.utexas.edu/, contact the Title IX Office via email at titleix@austin.utexas.edu, or call 512-471-0419. Although graduate teaching and research assistants are not subject to Texas Senate Bill 212, they are still mandatory reporters under Federal Title IX laws and are required to report a wide range of behaviors we refer to as sexual misconduct, including the types of sexual misconduct covered under Texas Senate Bill 212.The Title IX office has developed supportive ways to respond to a survivor and compiled campus resources to support survivors.

Faculty members and certain staff members are considered "Responsible Employees" or "Mandatory Reporters," which means that they are required to report violations of Title IX to the Title IX Coordinator. **I am a Responsible Employee and must report any Title IX-related incidents** that are disclosed in writing, discussion, or one-on-one. Before talking with me or with any faculty or staff member about a Title IX-related incident, be sure to ask whether they are a responsible employee. If you want to speak with someone for support or remedies without making an official report to the university, email advocate@austin.utexas.edu For more information about reporting options and resources, visit the Title IX Office or email titleix@austin.utexas.edu.

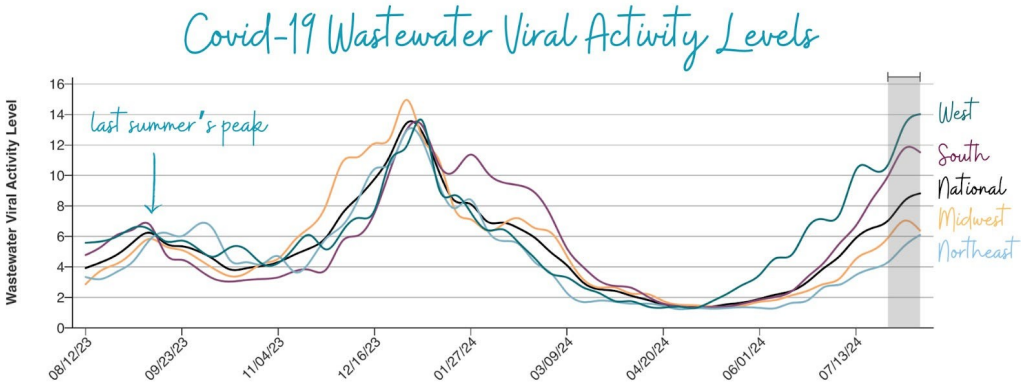
Doing your part to keep the Texas ChE community safe in the COVID-19 pandemic

Getting vaccinated + boosted reduces the chance of severe illness. You can be vaccinated at no cost, on campus and we strongly recommend doing so without delay.

Wearing a mask indoors, in class, and during activities will reduce the spread. N95 or similar masks are most effective.

Getting tested regularly can help prevent inadvertent spread of COVID-19. Testing is free and available whether you have COVID-19 symptoms or not. Rapid antigen tests may give false negatives, so also consider known exposures and any symptoms before engaging with others.

Staying home if you have symptoms, test positive, or were exposed to someone who tested positive helps end the chain of infectious spread.

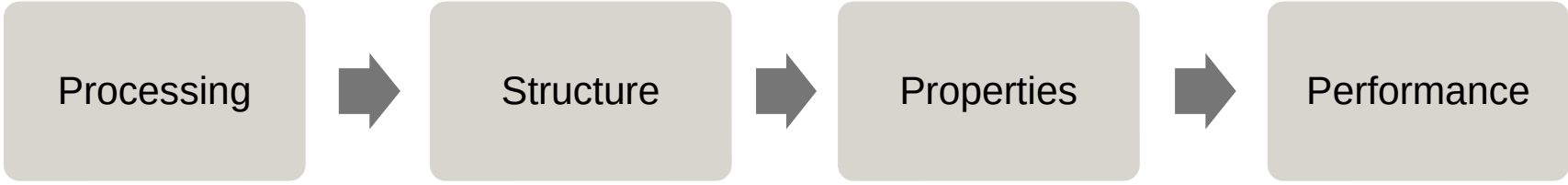


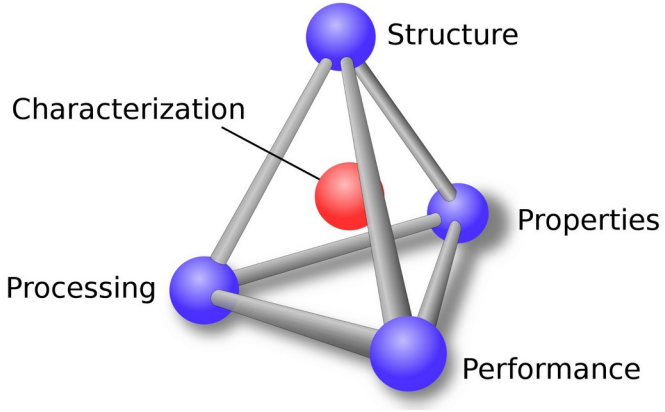
(Source: CDC; Annotations by YLE)

For more information visit protect.utexas.edu

What is materials science and engineering?

Discovering, understanding, and designing materials (often times solids) through the study and application of processing-structure-property-performance relationships

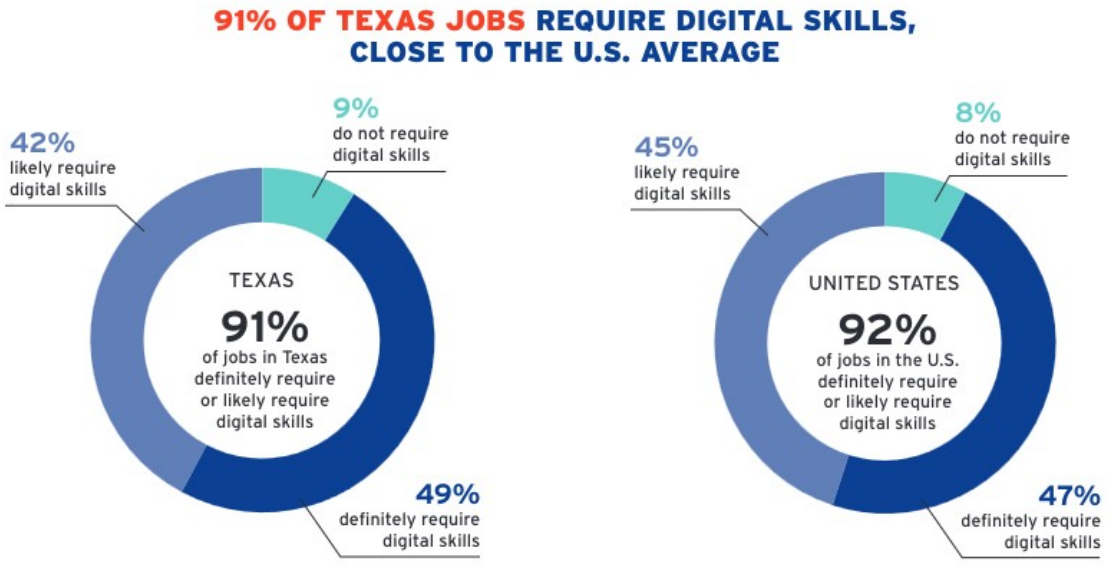




Why study computational materials science? (Think-pair-share)

Why study computational materials science? (Think-pair-share)

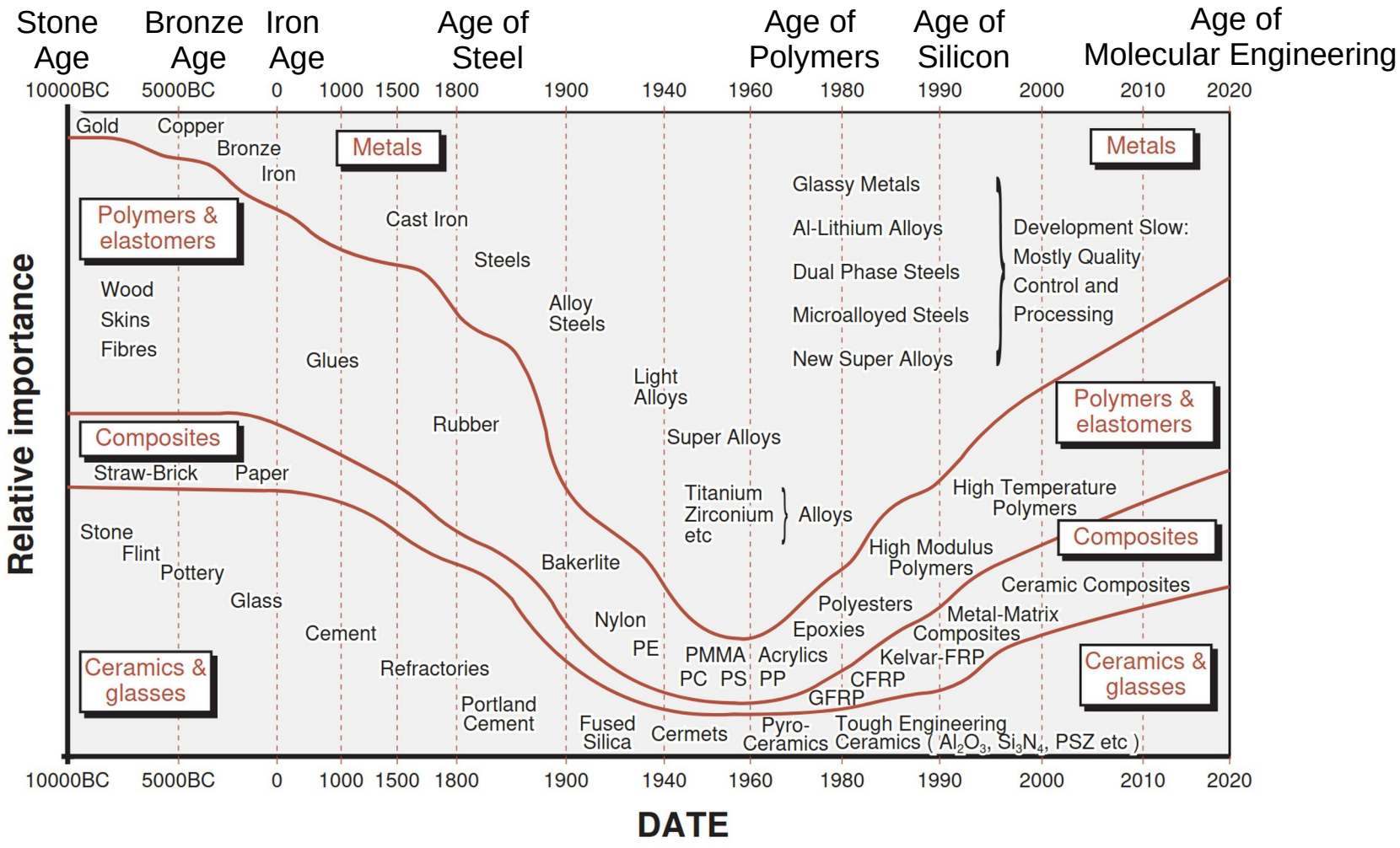
Digital v computational literacy



National Skills Coalition. Feb 2023

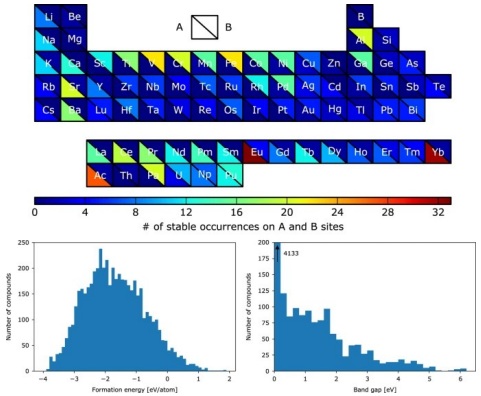
Between 2011 and 2021, STEM workforce grew 20%[1] and is projected to have one of the fastest growth rates

[1] NSF STEM Workforce Report, 2023



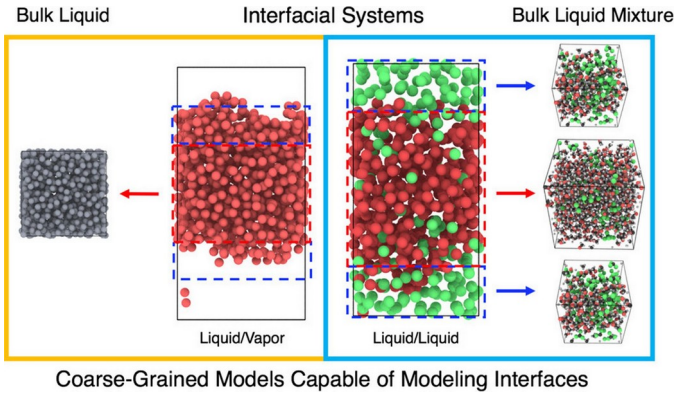
Adapted from Ashby M.F., 2005. Materials Selection in Mechanical Design, 3rd ed

Example of Computation in Materials Science and Engineering



Using supercomputers to discover new and ideal oxides

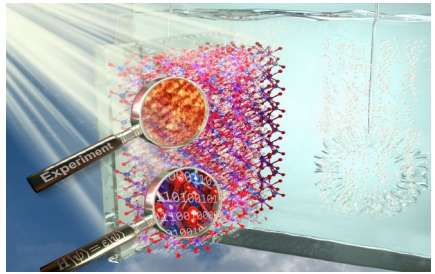
Wolverton Research Group, Northwestern



Coarse-Grained Models Capable of Modeling Interfaces

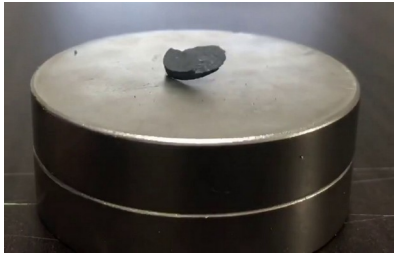
Interfacial phenomena through coarse-grained models

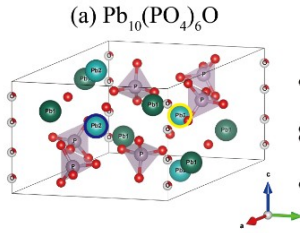
Voth Group, UChicago



Using defects to engineer optical and electronic properties

Wang Materials Group, UT Austin





LK-99 isn't a superconductor

Class introductions

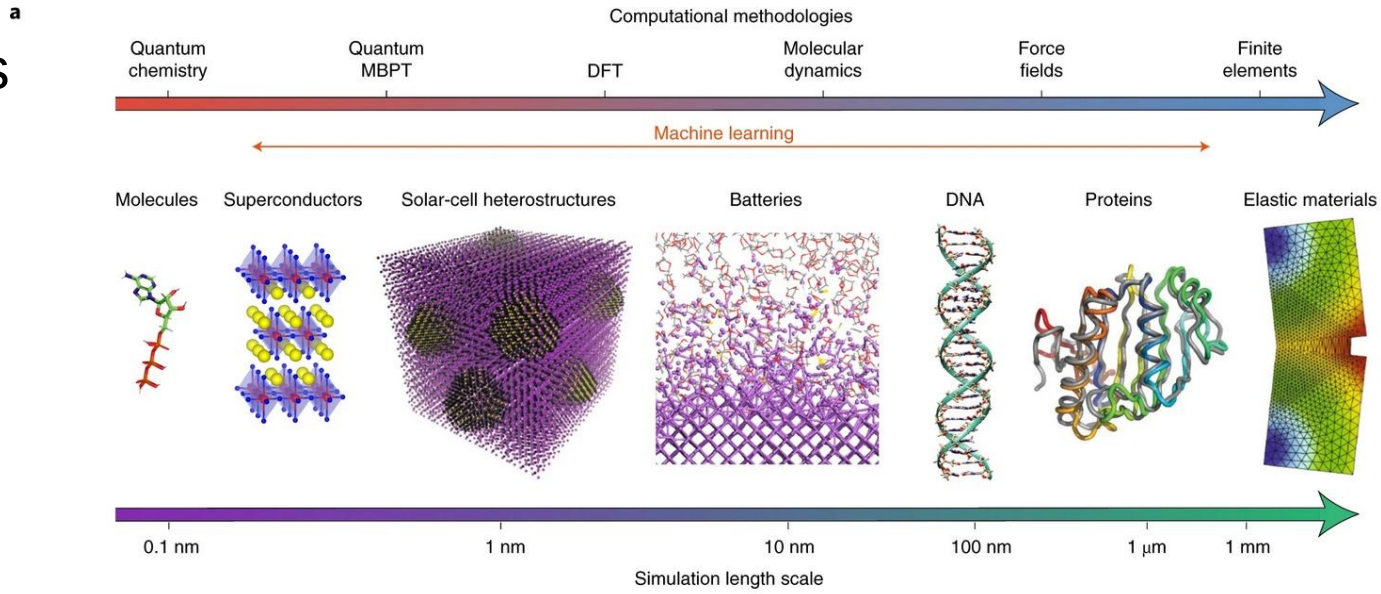
Name

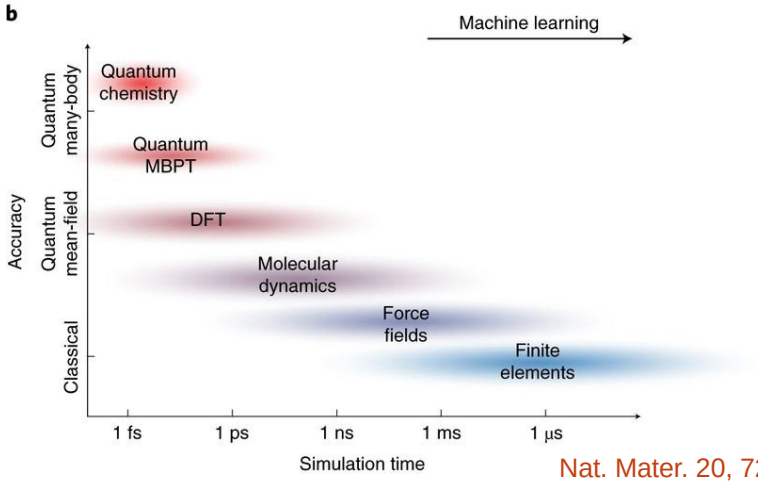
Year of study

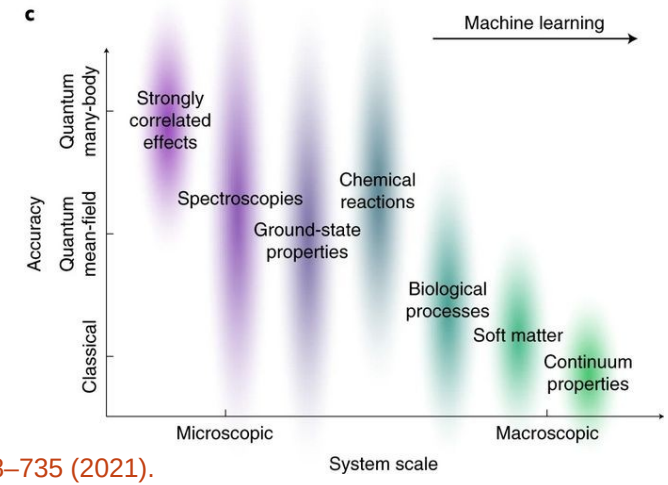
Department

An interesting factoid about yourself,
your research/academic interests, or
what you look forward to learning about in the course

Length and time scales in computational materials science



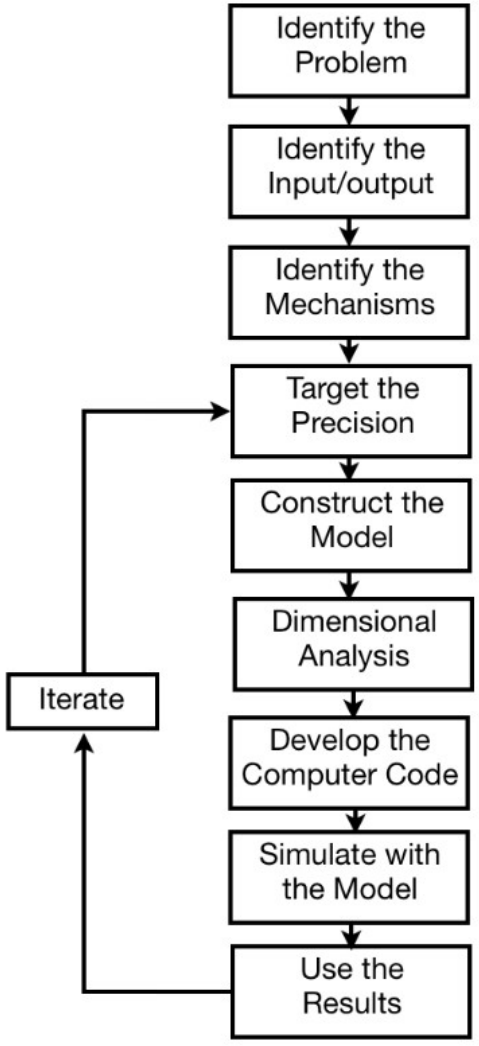




See also, Appendix A: Scientific units

Nat. Mater. 20, 728–735 (2021).

Developing a model



"Science and Statistics." George E.P. Box (1976)

"All models are wrong, but some are useful."

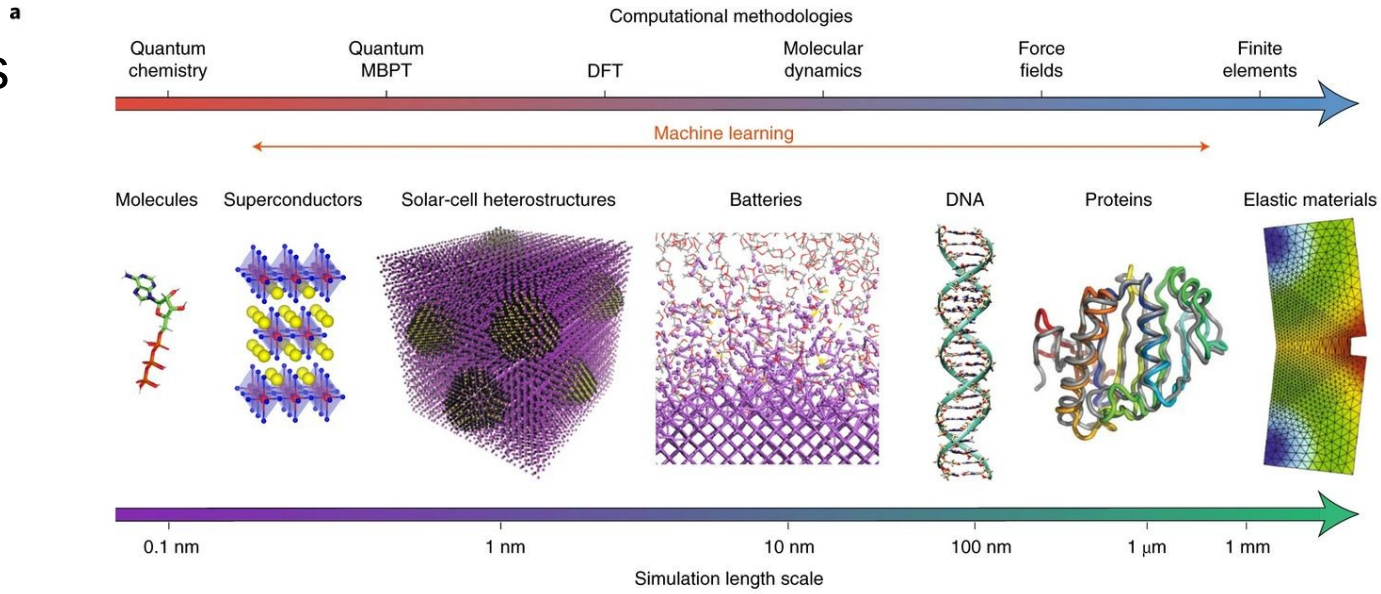
2.3 Parsimony

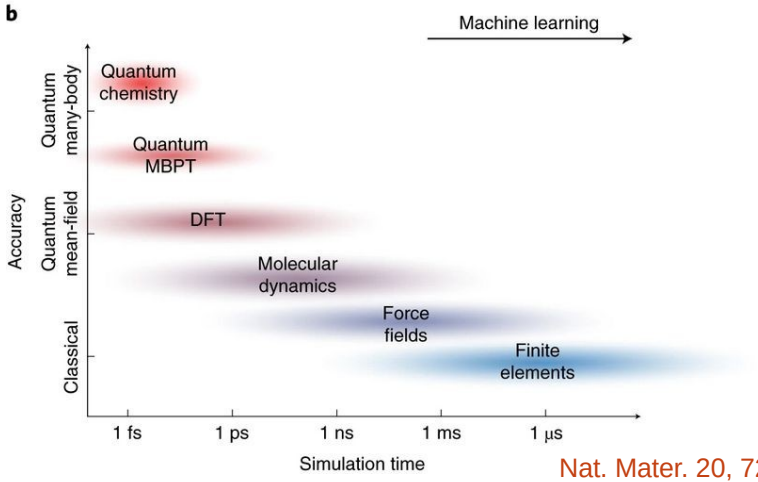
Since all models are wrong the scientist cannot obtain a "correct" one by excessive elaboration. On the contrary following William of Occam he should seek an economical description of natural phenomena. Just as the ability to devise simple but evocative models is the signature of the great scientist so overelaboration and overparameterization is often the mark of mediocrity.

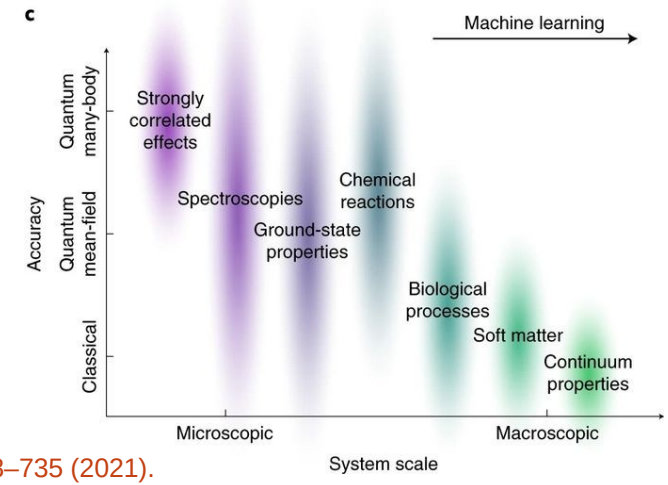
2.4 Worrying Selectively

Since all models are wrong the scientist must be alert to what is importantly wrong. It is inappropriate to be concerned about mice when there are tigers abroad.

Length and time scales in computational materials science







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