Welcome to
CHE 350: Chemical Engineering Materials

Introduction to Materials

Callister Ch 1

2023 MITE Summer Program

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

TEXAS MATERIALS INSTITUTE
Materials Science & Engineering

Lecture Outline

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

What is Materials Science and Engineering?

Examples

Materials Science Tetrahedron

Materials Classification

Materials Properties

What affects materials properties?

Next: Periodic trends

Typical first day

About this course

This course is an introduction to the fundamentals and application of materials science and engineering. 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. We will explore what this means in various systems, including metals, ceramics, polymers, and modern materials. Topics will include crystal structures, phase diagrams, diffusion, mechanical properties, and optoelectronic properties with an emphasis on structure-property-processing relationships.

Taken in 3rd or 4th year of ChE degree program

Goal: A foundational understanding of MS&E linked to applications

My background

Undergraduate

Materials Science & Engineering

MIT

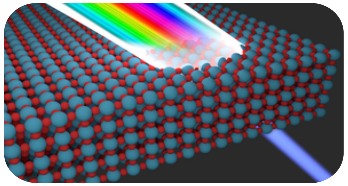
with
Prof. Brian Wardle
Mechanical testing of CNT aerospace composites

Graduate

Materials (Computation)

UC Santa Barbara

with
Prof. Chris G. Van de Walle
Electrochromism in complex oxides

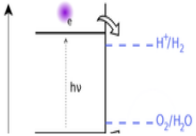


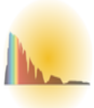
Post-doctoral

Molecular Engineering

University of Chicago

with
Prof. Giulia Galli &
Prof. Kyoung-Shin Choi
Materials optimization for photoelectrochemical water-splitting





wwwennie@che.utexas.edu | wangmaterialsgroup.com

Research Overview and Philosophy

DFT
MD
MBPT
$\hat{H}$ models
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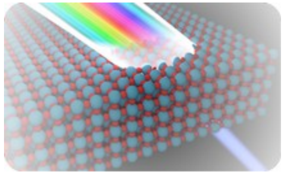
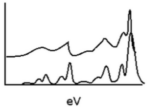
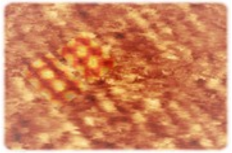
First-principles calculations



Enabled by HPC resources

Experimental collaboration





Spectroscopies, microscopies, ...

XPS
STM
XAS
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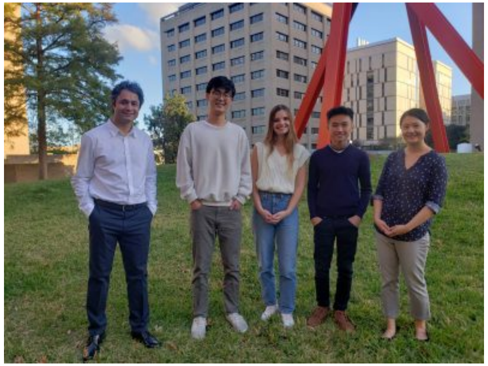
Harnessing Materials Imperfections for Energy Sustainability

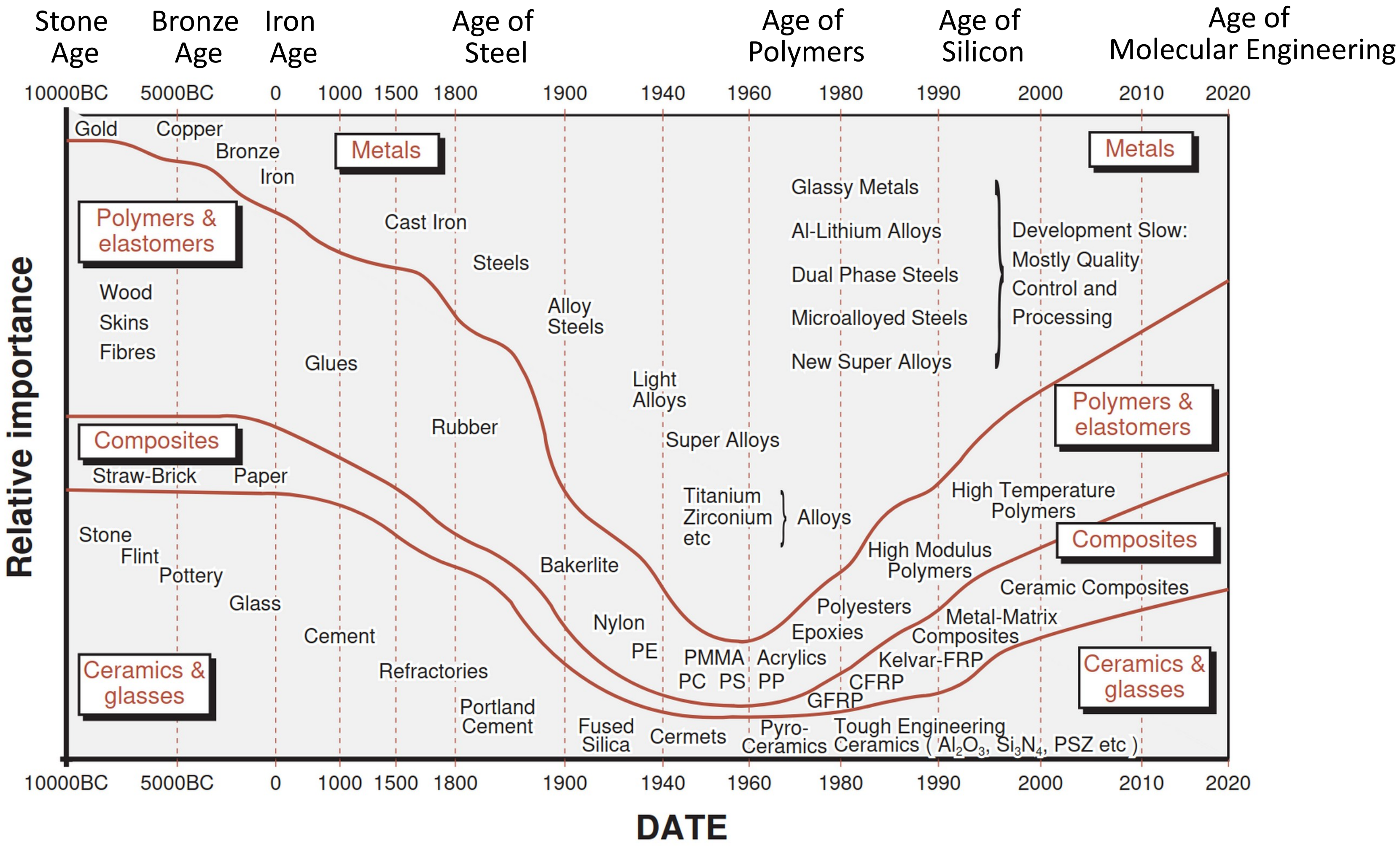


* Readings and supplementary materials will be posted periodically

* Subject to change

Class Topic	Reading (Callister)
Introduction to Materials	Ch 1
Atomic Structure and Interatomic Interactions	Ch 2
Crystallographic systems, directions, planes	Ch 3, parts of Ch 12
XRD and Diffraction	Ch 3
Crystallographic defects	Ch 4
Diffusion in solids	Ch 5
Exam: Wednesday 02/08	
Nucleation and Kinetics	parts of Ch 10
Mechanical Properties of metals and ceramics	Ch 6, parts of Ch 7 & 12
Materials failure- fracture	Ch 8
Materials failure- corrosion	Ch 17
Phase diagrams and phase transformations	Ch 9
Exam: Wednesday 03/08	
Polymers: structure, properties, and synthesis	Ch 14 and 15
Electronic structure	
Electronic properties	Ch 18
Exam: Wednesday 04/12	
Optical properties of materials	Ch 21
Optoelectronic devices- pn junctions	Supplemented Ch 18
Materials and the Environment	Ch 22
Final Exam, Thursday 04/27, 1:00-3:00 pm	

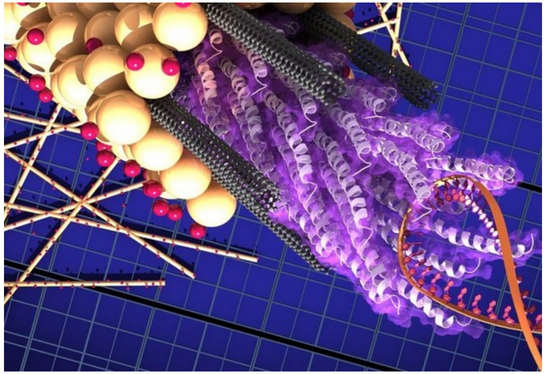
Why study materials? (Think-pair-share)



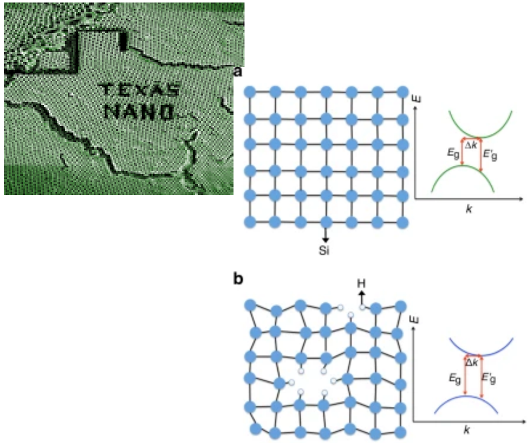
Adapted from Ashby M.F., 2005. Materials Selection in Mechanical Design, 3rd ed

Examples of Materials Science and/or Engineering

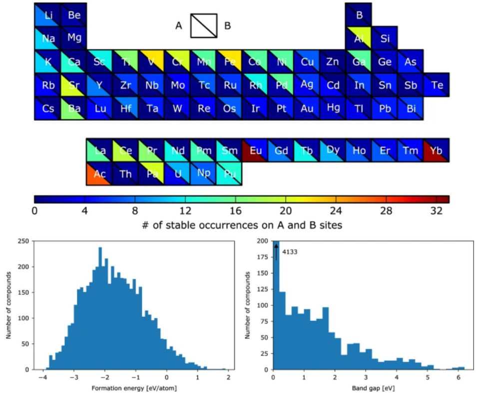
3D printing soft bio-polymers
Nelson Lab, University of Washington



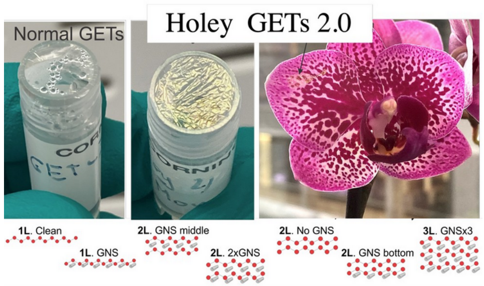
Using viruses as templates to
make more efficient solar cells
Belcher Lab, MIT



Using defects in nanoparticles for high-
efficiency, low-loss nanophotonics
Korgel & Zheng Research Groups, UT Austin

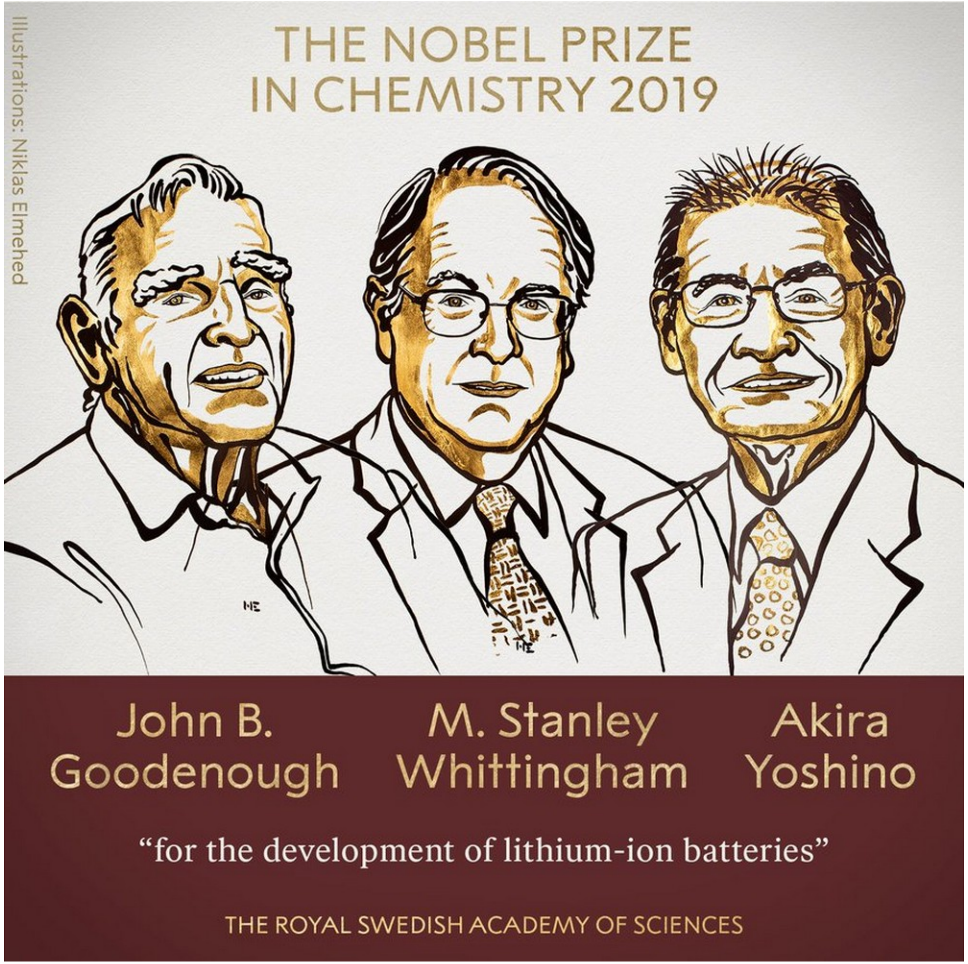


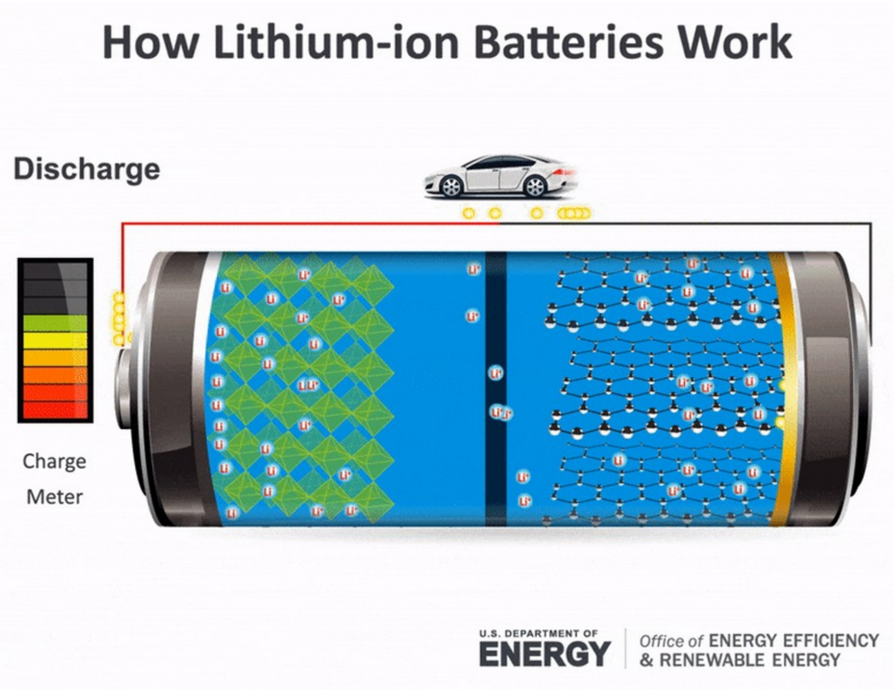
Using supercomputers to discover
new and ideal oxides
Wolverton Research Group, Northwestern



Breathable graphene tatoos
for personalized healthcare
Akinwande Nano Research Group, UT Austin

What is the materials science behind Li-ion battery winning the 2019 Nobel prize in Chemistry?





Why can plastics only be recycled a limited number of times but glass and metal can be recycled without limit?

Image from Murphy, L. Earth911 (2020)

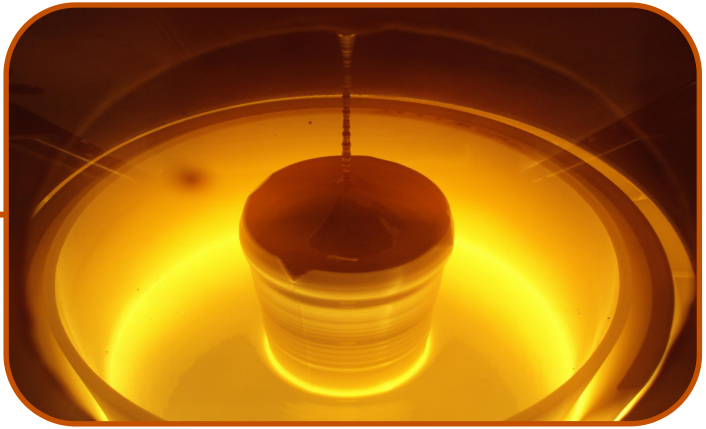
What is materials science and engineering?

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

Processing → Structure → Properties → Performance

What is materials science and engineering?

How is the material actually made in a lab/factory or adapted from nature?

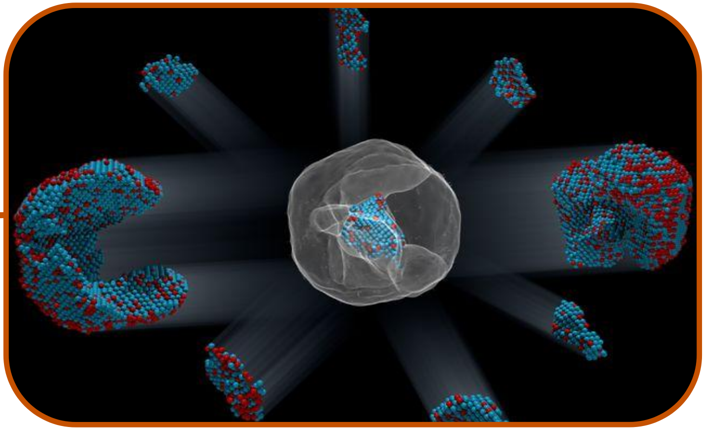


Processing → Structure → Properties → Performance

Adapted from Modern Materials Technologies, Image from Omnidyne

What is materials science and engineering?

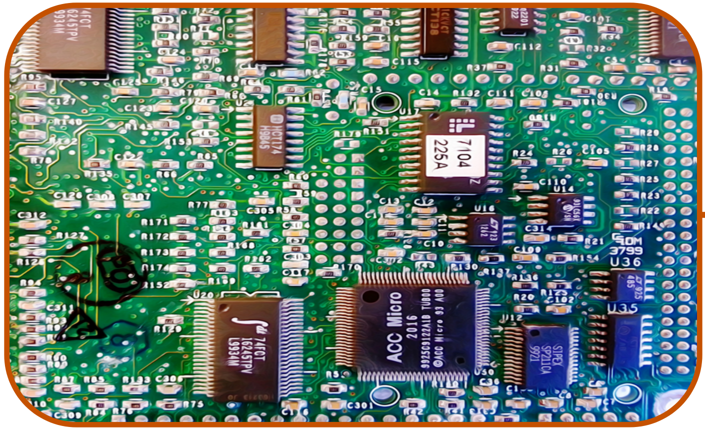
How are the internal components arranged?



Processing → Structure → Properties → Performance

Adapted from Modern Materials Technologies, Image from Chong, L. "Bringing atomic mapping to the mainstream" Phys Org (2017)

What is materials science and engineering?



How does it respond to an external stimulus?

Mechanical

Electrical

Thermal

Magnetic

Optical

Chemical

Processing → Structure → Properties → Performance

Adapted from Modern Materials TechnologiesModern Materials Technologies

What is materials science and engineering?

How does the material help the user/world?

Processing → Structure → Properties → Performance

Image from Alset International

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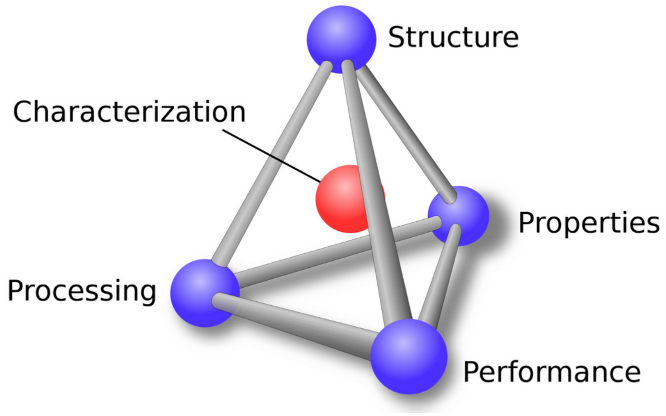

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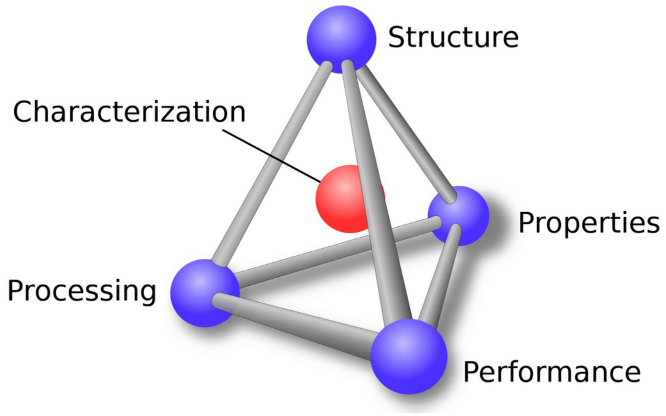


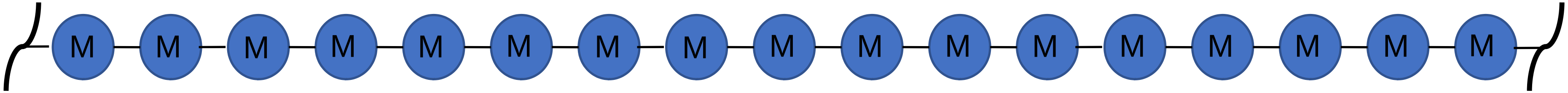
Why can plastics only be recycled a limited number of times but glass and metal can be recycled (theoretically) without limit?

Image from Murphy, L. Earth911 (2020)

Why study polymers?

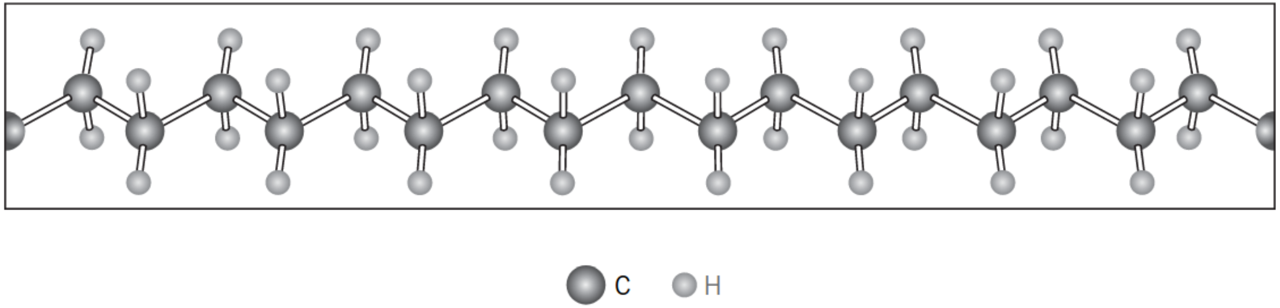
https://www.youtube.com/watch?v=UwRVj9rz2QQ

Polymers: what are they

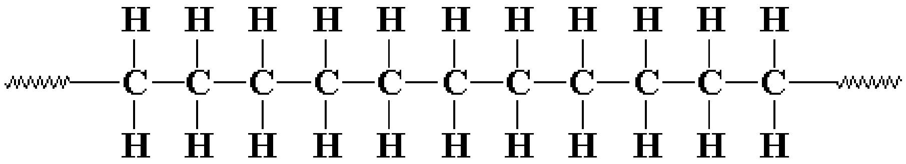


Polymers are a special type of molecule that are made up of simple building blocks called **monomers…**

…that **bond** together in a **repeating pattern** to form very large **macromolecules.**



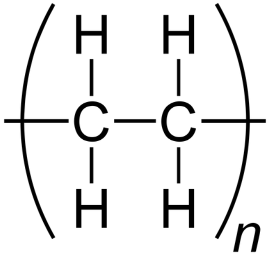
Polymers: what are they?



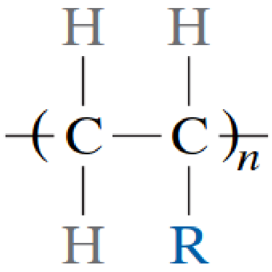
Make n-chain and get polyethylene, the simplest organic **polymer**

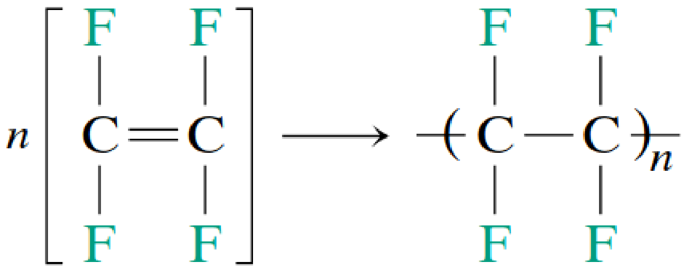
This is a widely used plastic!

We abbreviate polymers with monomer unit notation

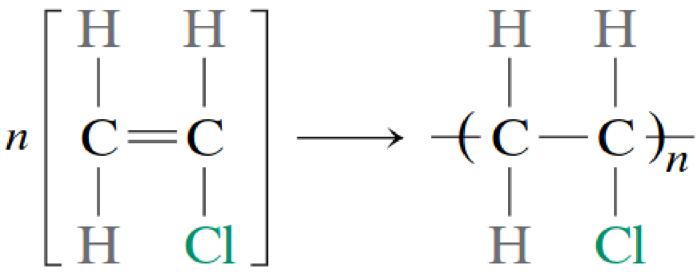


Tuning composition with side groups R





Polytetrafluoroethylene (Teflon)



Polyvinylchloride (PVC)

In-class crafting: Polymer structure and processing

Characterizing Polymers: Molecular Structure and bonding

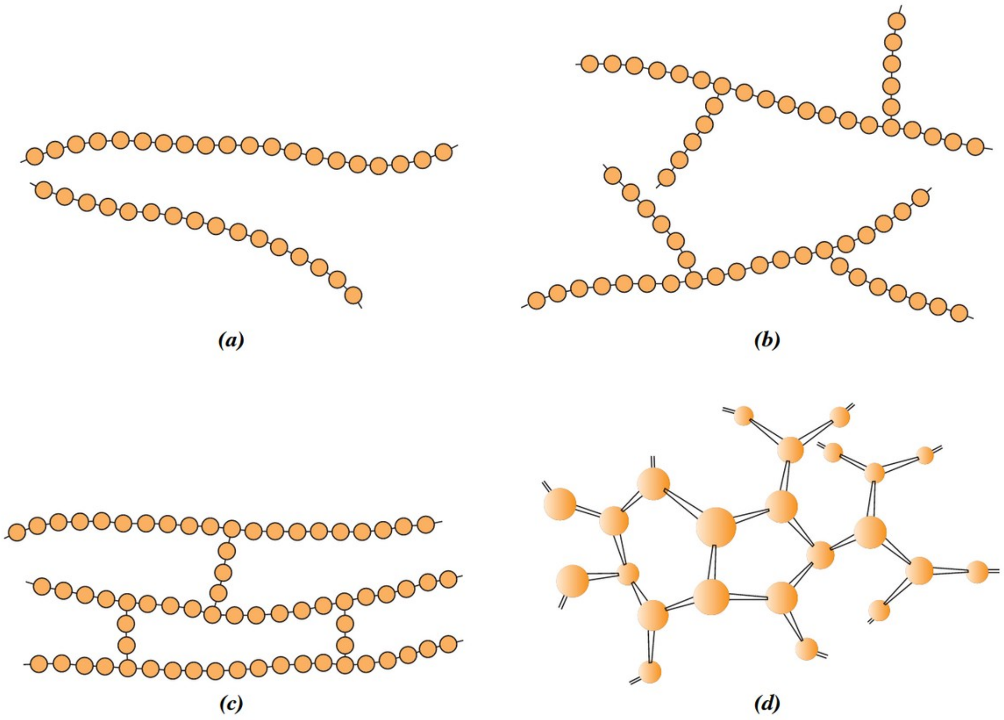
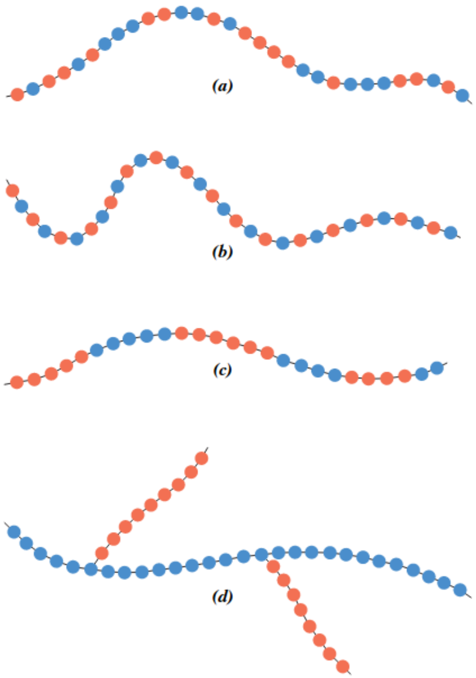


Figure 14.7 Schematic representations of (*a*) linear, (*b*) branched, (*c*) crosslinked, and (*d*) network (three-dimensional) molecular structures. Circles designate individual repeat units.

Figure 14.9 Schematic representations of (*a*) random, (*b*) alternating, (*c*) block, and (*d*) graft copolymers. The two different repeat unit types are designated by blue and red circles.



In-class crafting: Polymer structure and processing

Polyclip #1	Alternating co-polymer
Polyclip #2	Branched polymer
Polyclip #3	Graft co-polymer
Polyclip #4	Linear polymer
Polyclip #5	Cross-linked polymer
Polyclip #6	Random co-polymer

The Periodic Table is our playground