



# 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



# 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 3<sup>rd</sup> or 4<sup>th</sup> 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



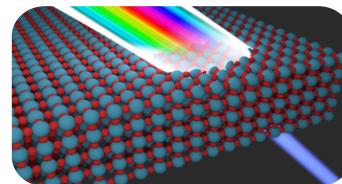
## Graduate

Materials (Computation)

UC Santa Barbara

with

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



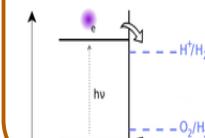
## Post-doctoral

Molecular Engineering

University of Chicago

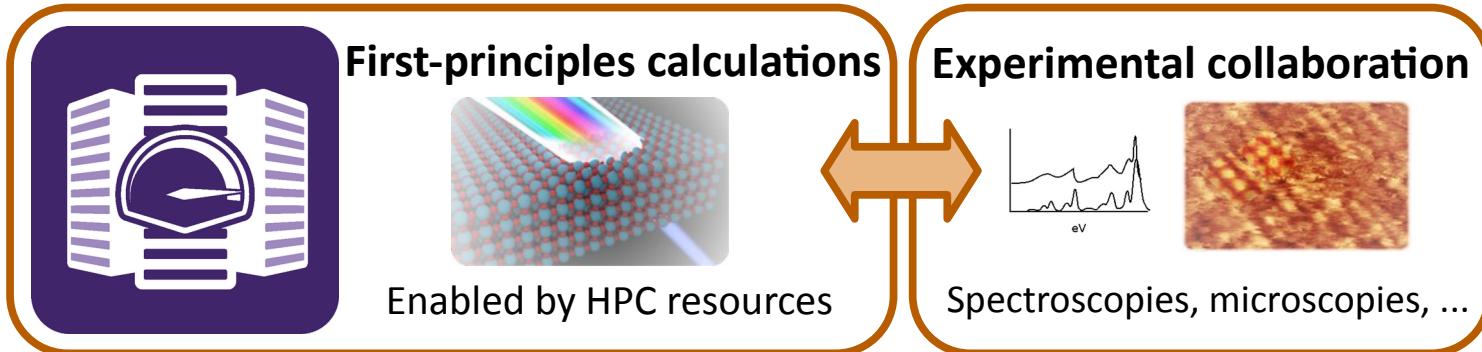
with

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

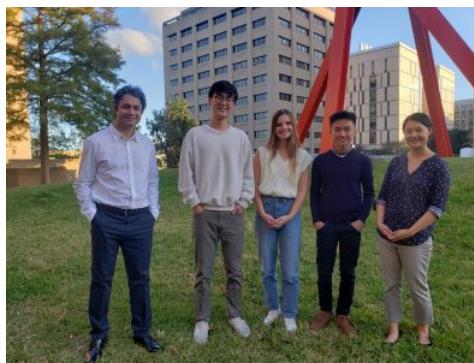


# Research Overview and Philosophy

DFT  
MD  
MBPT  
 $\hat{H}$  models  
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## Harnessing Materials Imperfections for Energy Sustainability

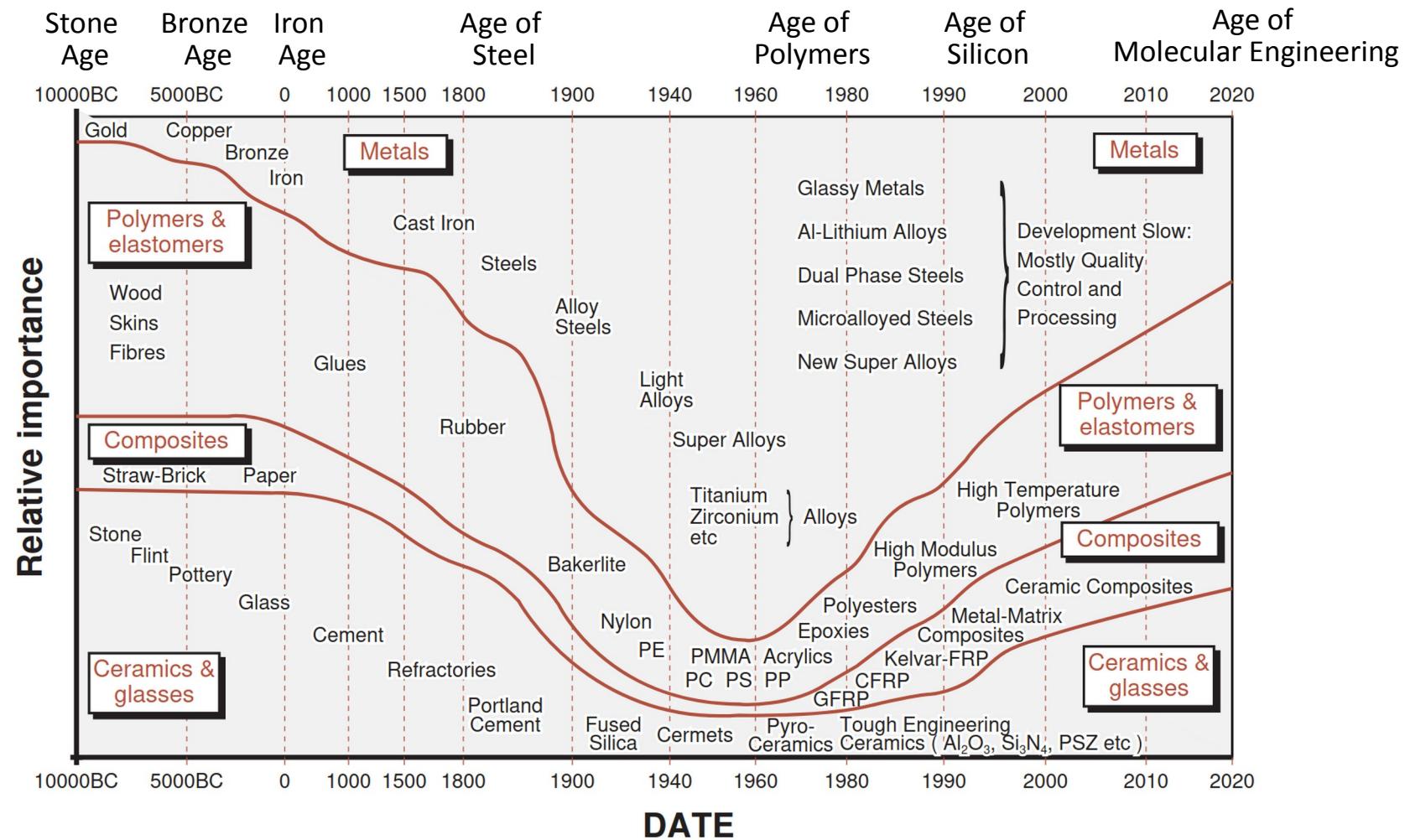


\* Readings and supplementary materials will be posted periodically

\* 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
<b>Exam: Wednesday 02/08</b>	
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
<b>Exam: Wednesday 03/08</b>	
Polymers: structure, properties, and synthesis	Ch 14 and 15
Electronic structure	
Electronic properties	Ch 18
<b>Exam: Wednesday 04/12</b>	
Optical properties of materials	Ch 21
Optoelectronic devices- pn junctions	Supplemented Ch 18
Materials and the Environment	Ch 22
<b>Final Exam, Thursday 04/27, 1:00-3:00 pm</b>	

# Why study materials? (Think-pair-share)



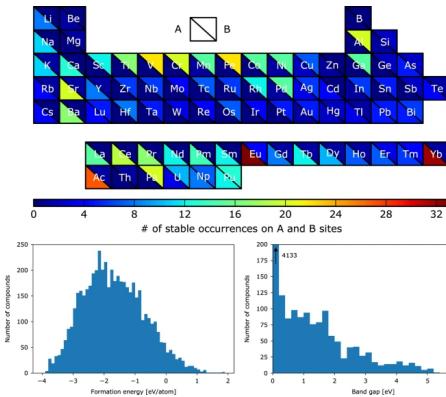
# Examples of Materials Science and/or Engineering



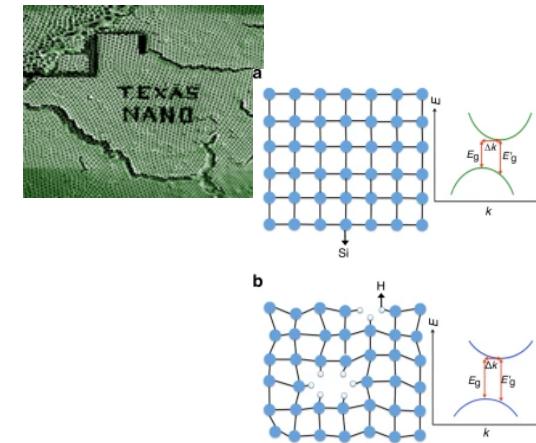
3D printing soft bio-polymers  
Nelson Lab, University of Washington



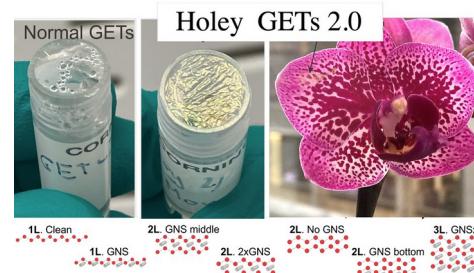
Using viruses as templates to  
make more efficient solar cells  
Belcher Lab, MIT



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



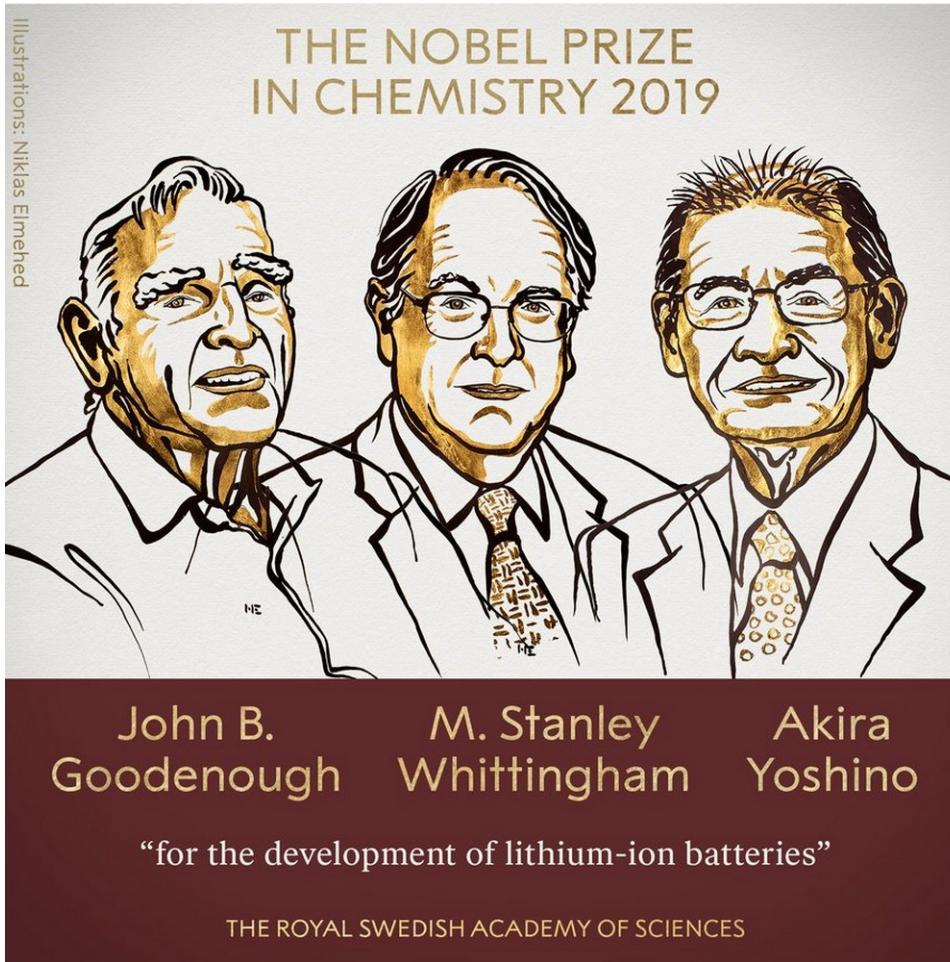
Using defects in nanoparticles for high-  
efficiency, low-loss nanophotonics  
Korgel & Zheng Research Groups, UT Austin



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

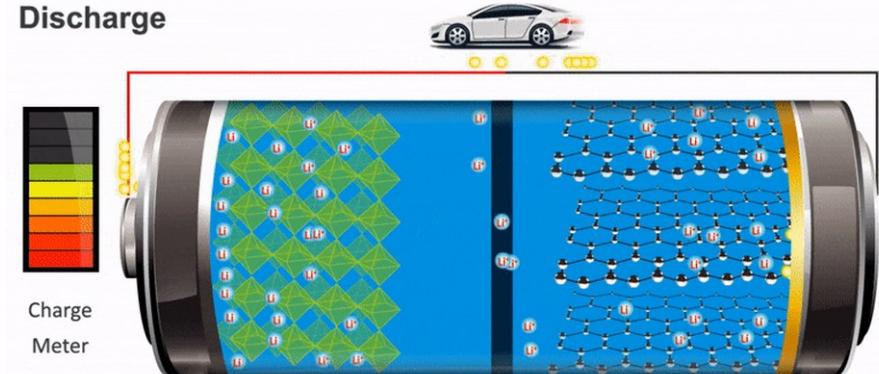
# What is the materials science behind Li-ion battery winning the 2019 Nobel prize in Chemistry?

Illustrations: Niklas Elmehed



## How Lithium-ion Batteries Work

Discharge

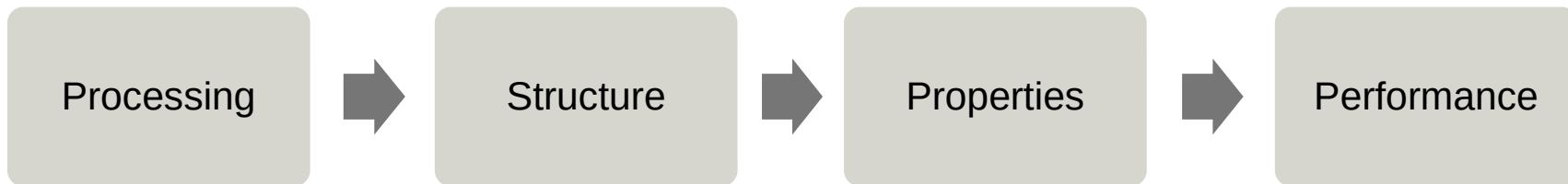


Why can plastics only be recycled a limited number of times  
but glass and metal can be recycled without limit?

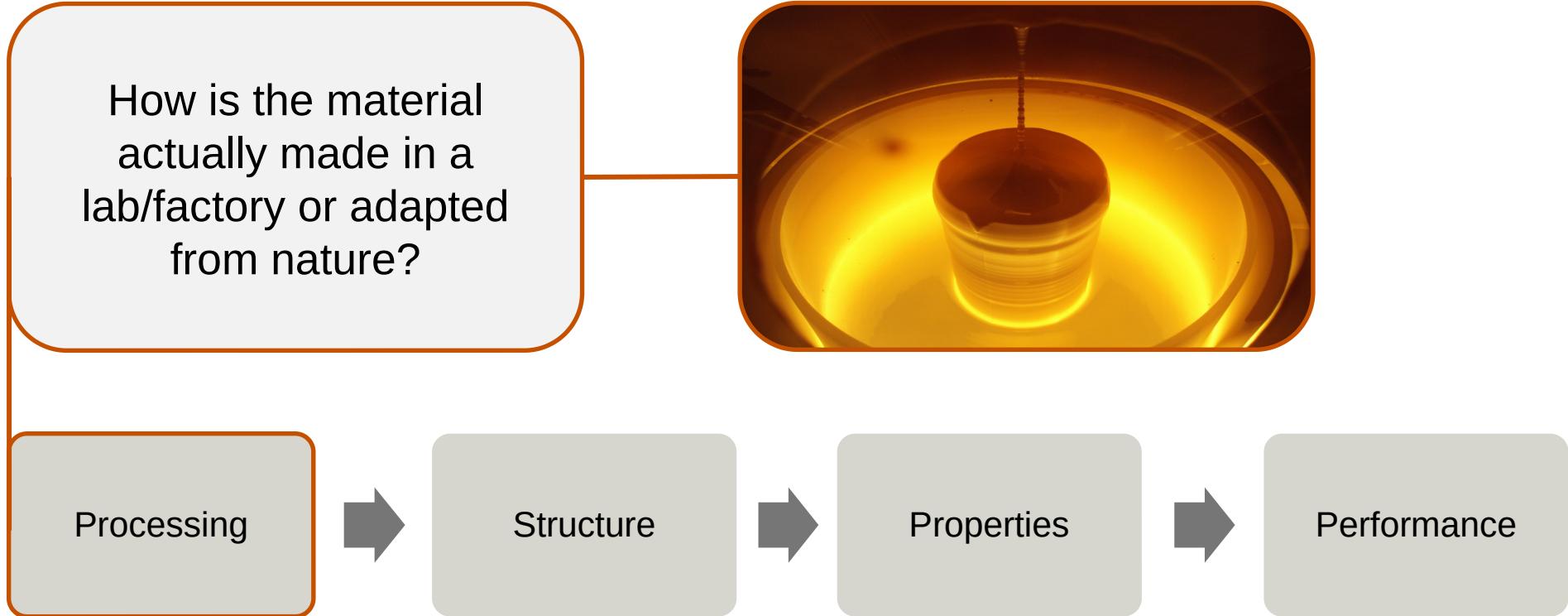


# What is materials science and engineering?

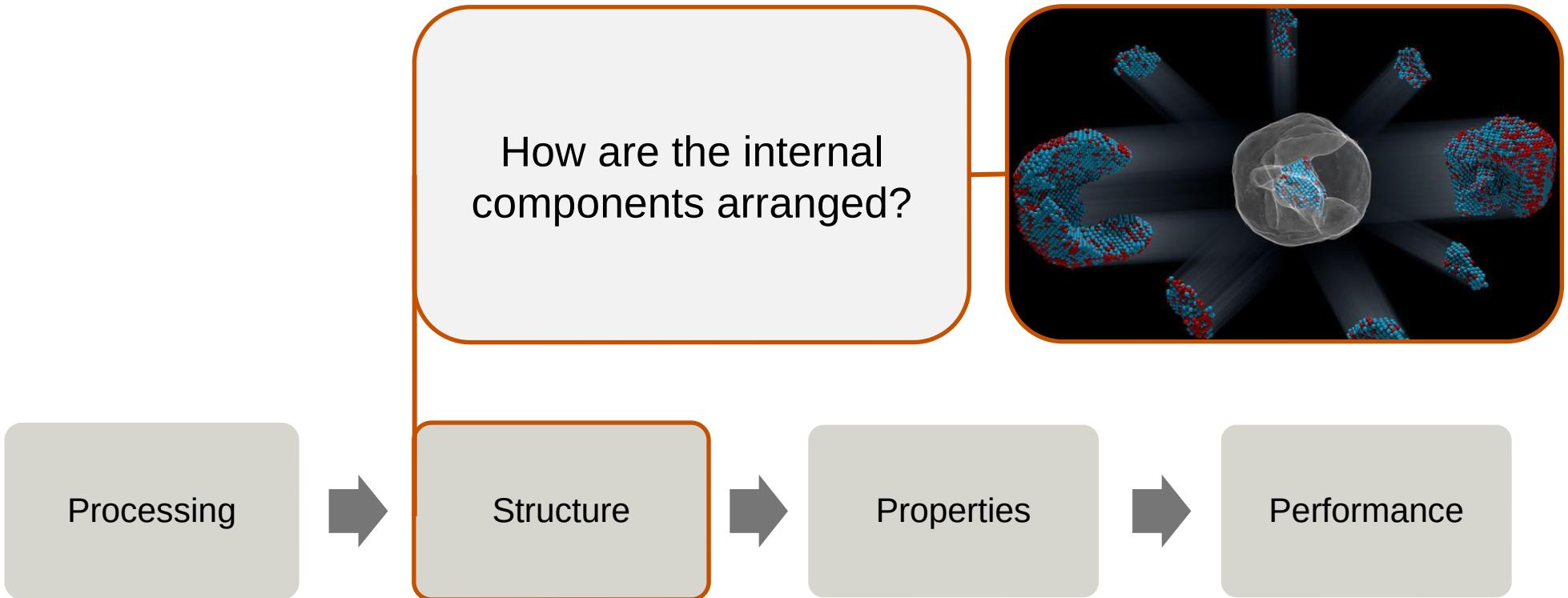
Discovering, understanding, and designing materials (often times solids) through the study and application of processing-structure-property-performance relationships



# What is materials science and engineering?



# What is materials science and engineering?



# What is materials science and engineering?



How does it respond to an external stimulus?

Mechanical

Electrical

Thermal

Magnetic

Optical

Chemical

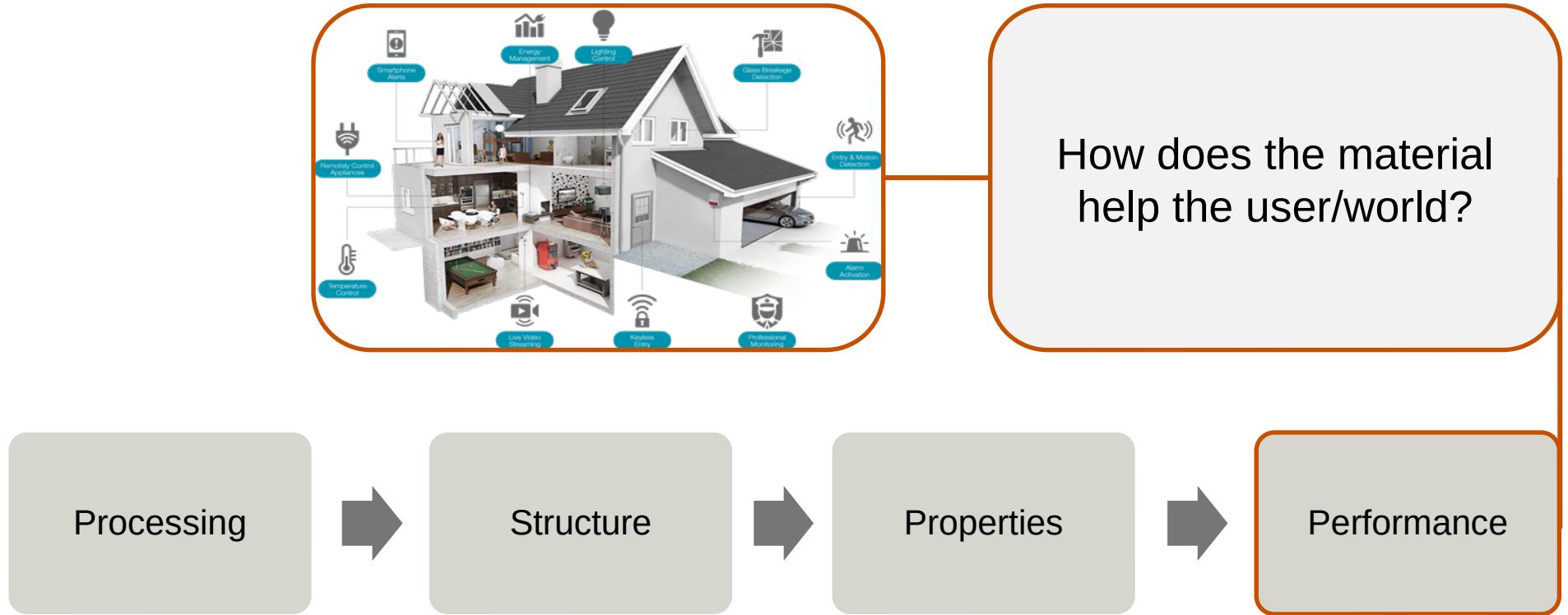
Processing

Structure

Properties

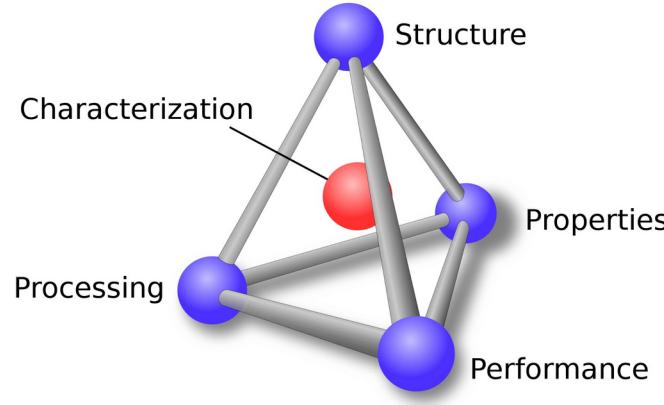
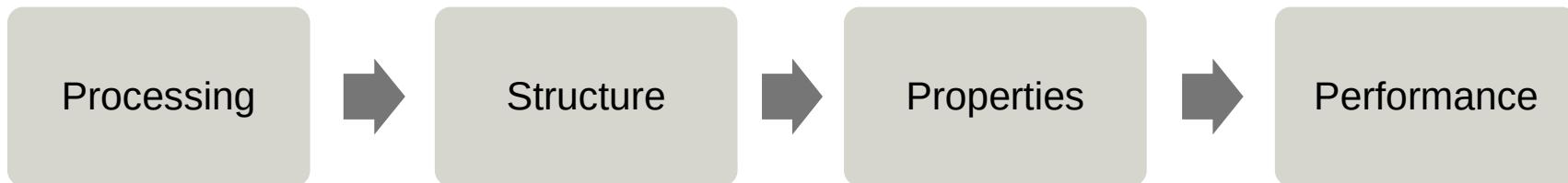
Performance

# What is materials science and engineering?

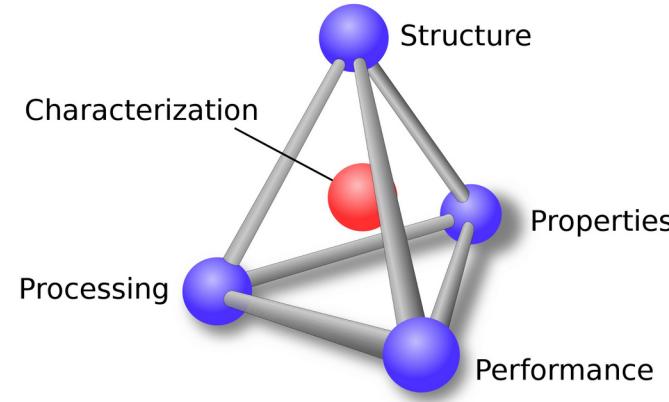
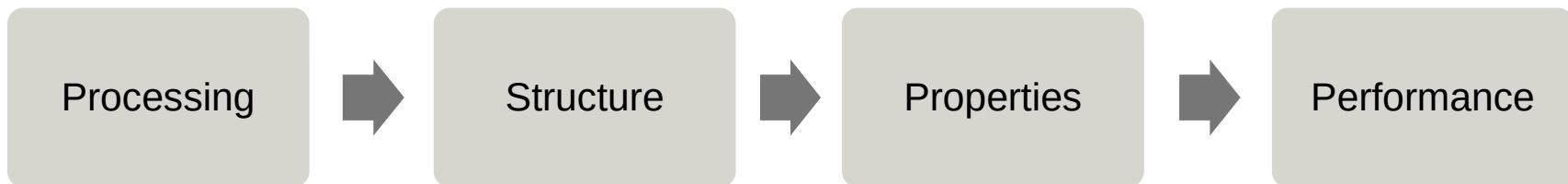


# What is materials science and engineering?

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



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



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

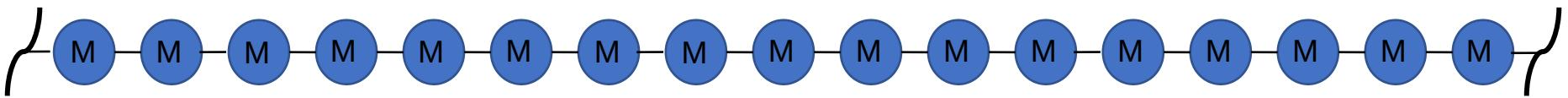


# Why study polymers?



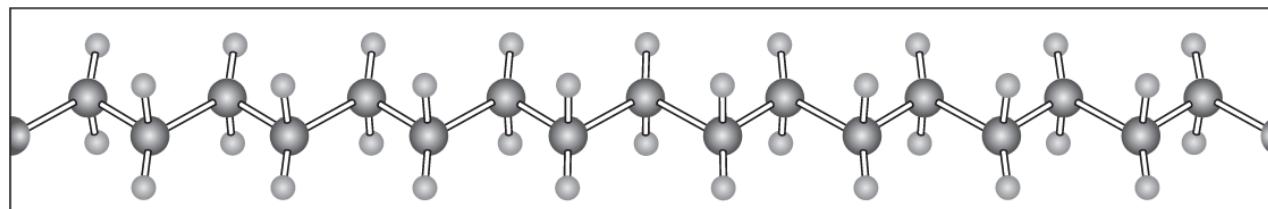
<https://www.youtube.com/watch?v=UwRVj9rz2QQ>

# Polymers: what are they



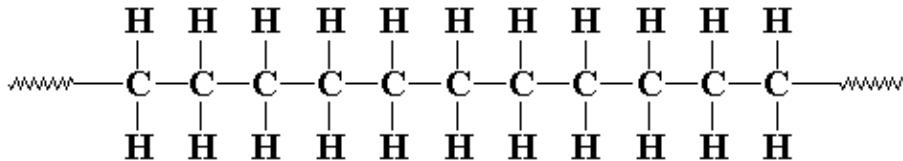
Polymers are a special type of molecule that are made up of simple building blocks called **monomers**...

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



● C   ● H

# Polymers: what are they?

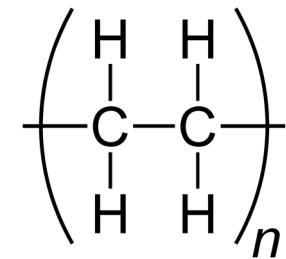


Make n-chain and get polyethylene, the simplest organic **polymer**

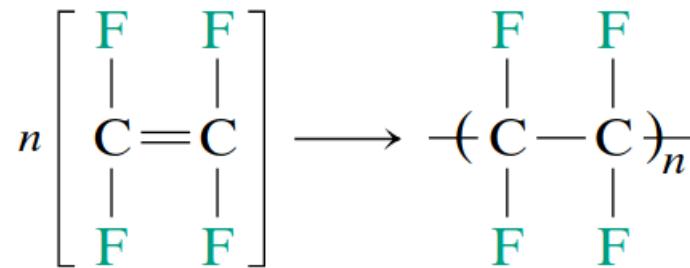
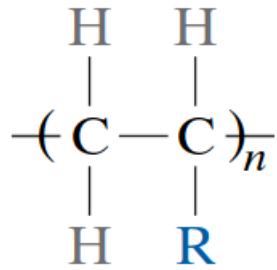
This is a widely used plastic!



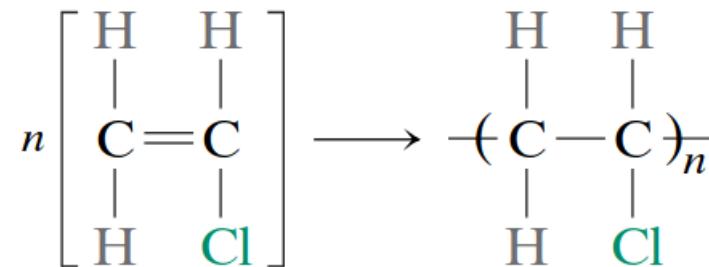
We abbreviate polymers with monomer unit notation



# Tuning composition with side groups R



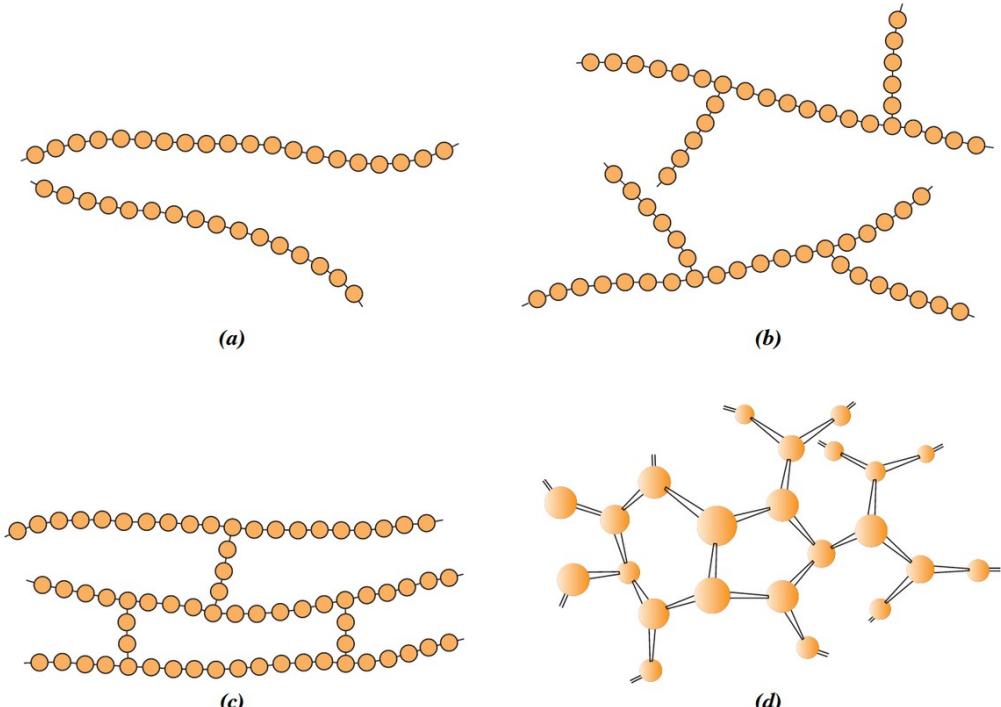
**Polytetrafluoroethylene (Teflon)**



**Polyvinylchloride (PVC)**

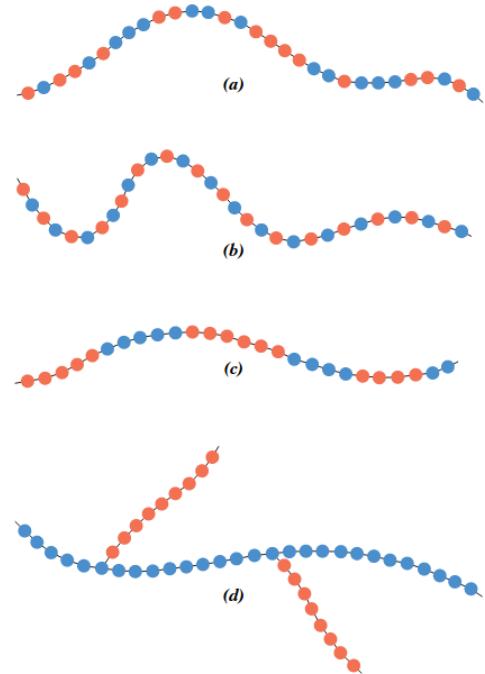
# In-class crafting: Polymer structure and processing

# 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

1	H	He
	Hydrogen	Helium
3	Li	Be
	Lithium	Beryllium
11	Na	Mg
	Sodium	Magnesium
19	K	Ca
	Potassium	Calcium
37	Rb	Sr
	Rubidium	Strontium
55	Cs	Ba
	Caesium	Barium
87	Fr	Ra
	Francium	Radium
4	Be	
	Beryllium	
12	Mg	
	Magnesium	
20	Ca	Sc
	Calcium	Scandium
38	Sr	Y
	Strontium	Yttrium
56	Ba	La
	Barium	Lanthanum
88	Ra	
	Radium	
89	Ac	
	Actinium	
22	Ti	V
	Titanium	Vanadium
23	Cr	Mn
	Chromium	Manganese
24	Fe	Co
	Iron	Cobalt
25	Mn	Ni
	Manganese	Nickel
26	Fe	Cu
	Iron	Copper
27	Co	Zn
	Cobalt	Zinc
28	Ni	
	Nickel	
29	Cu	
	Copper	
30	Zn	
	Zinc	
31	Ga	Al
	Gallium	Aluminum
32	Ge	Si
	Germanium	Silicon
33	As	P
	Arsenic	Phosphorus
34	Se	S
	Selenium	Sulfur
35	Br	Cl
	Bromine	Chlorine
36	Kr	
	Krypton	
37	Rb	Sr
	Rubidium	Strontium
38	Sr	Y
	Strontium	Yttrium
39	Y	
	Yttrium	
40	Zr	Nb
	Zirconium	Niobium
41	Mo	Tc
	Molybdenum	Technetium
42	Tc	Ru
	Technetium	Ruthenium
43	Ru	Rh
	Ruthenium	Rhodium
44	Rh	Pd
	Rhodium	Palladium
45	Pd	Ag
	Palladium	Silver
46	Ag	Cd
	Silver	Cadmium
47	Cd	In
	Cadmium	Indium
48	In	
	Indium	
49	Sn	Sb
	Tin	Antimony
50	Sb	Te
	Antimony	Tellurium
51	Te	I
	Tellurium	Iodine
52	I	
	Iodine	
53	Xe	
	Xenon	
54	Rn	
	Radon	
55	Cs	Ba
	Caesium	Barium
56	Ba	La
	Barium	Lanthanum
57	La	
	Lanthanum	
72	Hf	Ta
	Hafnium	Tantalum
73	Ta	W
	Tantalum	Tungsten
74	W	Re
	Tungsten	Rhenium
75	Re	Os
	Rhenium	Osmium
76	Os	Ir
	Osmium	Iridium
77	Ir	Pt
	Iridium	Platinum
78	Pt	Au
	Platinum	Gold
79	Au	Hg
	Gold	Mercury
80	Hg	
	Mercury	
81	Tl	Pb
	Thallium	Lead
82	Pb	Bi
	Lead	Bismuth
83	Bi	Po
	Bismuth	Polonium
84	Po	At
	Polonium	Astatine
85	At	
	Astatine	
86	Rn	
	Radon	
104	Rf	Db
	Rutherfordium	Dubnium
105	Db	Sg
	Dubnium	Seaborgium
106	Sg	Bh
	Seaborgium	Bohrium
107	Bh	Hs
	Bohrium	Hassium
108	Hs	Mt
	Hassium	Meitnerium
109	Mt	Ds
	Meitnerium	Darmsta...
110	Ds	Rg
	Darmsta...	Roentgenium
111	Rg	Cn
	Roentgenium	Copernic...
112	Cn	
	Copernic...	
113	Nh	Fl
	Nihonium	Flerovium
114	Fl	Mc
	Flerovium	Moscovium
115	Mc	Lv
	Moscovium	Livermorium
116	Lv	Ts
	Livermorium	Tenness...
117	Ts	Og
	Tenness...	Oganesson
58	Ce	Pr
	Cerium	Praseodymium
59	Pr	Nd
	Praseodymium	Neodymium
60	Nd	Pm
	Neodymium	Promethium
61	Pm	Sm
	Promethium	Samarium
62	Sm	Eu
	Samarium	Europium
63	Eu	Gd
	Europium	Gadolinium
64	Gd	Tb
	Gadolinium	Terbium
65	Tb	Dy
	Terbium	Dysprosium
66	Dy	Ho
	Dysprosium	Holmium
67	Ho	Er
	Holmium	Erbium
68	Er	Tm
	Erbium	Thulium
69	Tm	Yb
	Thulium	Ytterbium
70	Yb	Lu
	Ytterbium	Lutetium
71	Lu	
	Lutetium	
90	Th	Pa
	Thorium	Protactinium
91	Pa	U
	Protactinium	Uranium
92	U	Np
	Uranium	Neptunium
93	Np	Pu
	Neptunium	Plutonium
94	Pu	Am
	Plutonium	Americium
95	Am	Cm
	Americium	Curium
96	Cm	Bk
	Curium	Berkelium
97	Bk	Cf
	Berkelium	Californium
98	Cf	Es
	Californium	Einsteinium
99	Es	Fm
	Einsteinium	Fermium
100	Fm	Md
	Fermium	Mendeleevium
101	Md	No
	Mendeleevium	Nobelium
102	No	Lr
	Nobelium	Lawrencium

- Alkali metals
  - Alkaline earth metals
  - Transition metals
  - Post-transition metals
  - Metalloids
  - Reactive nonmetals
  - Noble gases
  - Lanthanides
  - Actinides
  - Unknown properties