Day 3:
YALE PATHWAYS TO SCIENCE SUMMER WORKSHOP 2021

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Introduction to Materials Science

DESIGN OF NEW MATERIALS USING SUPERCOMPUTERS

LEARNING GOALS

- What is a material? Why is it important to study Materials Science?
- What is a crystal and its unit-cell?
- What is a defect? Why is it important?

DEFINITION OF A MATERIAL

- Activity: Name an object/material you can see around you?

Can you tell what it is made of?

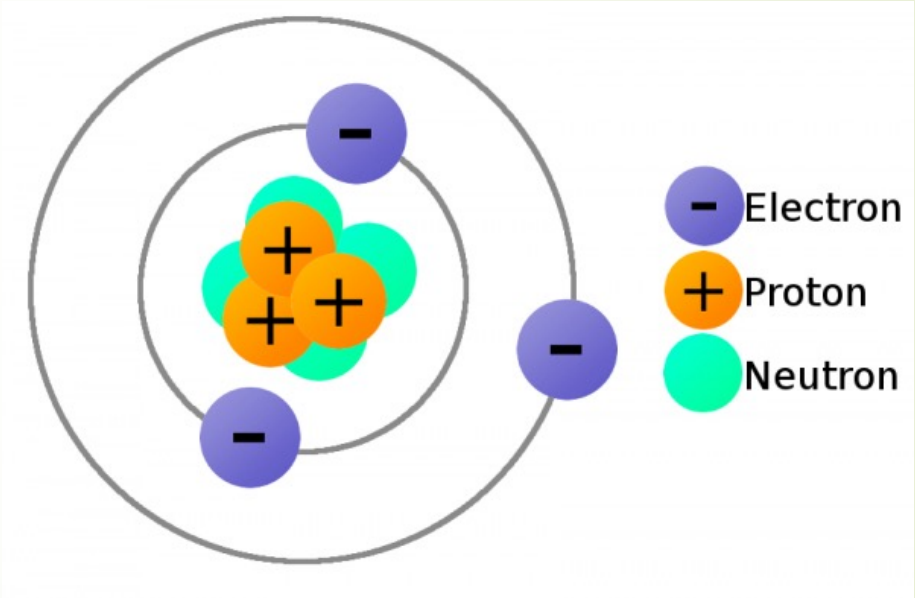
- QUIZ: Which of the following is an element?

A) Wood

B) Steel

C) Salt

D) Iron



- An element is a pure substance that has atoms with the same number of protons in its nuclei

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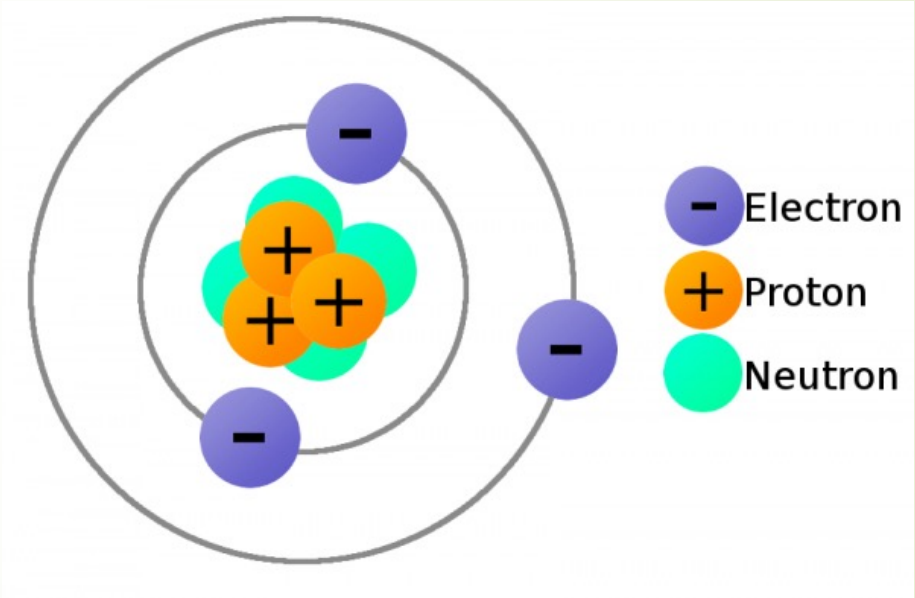

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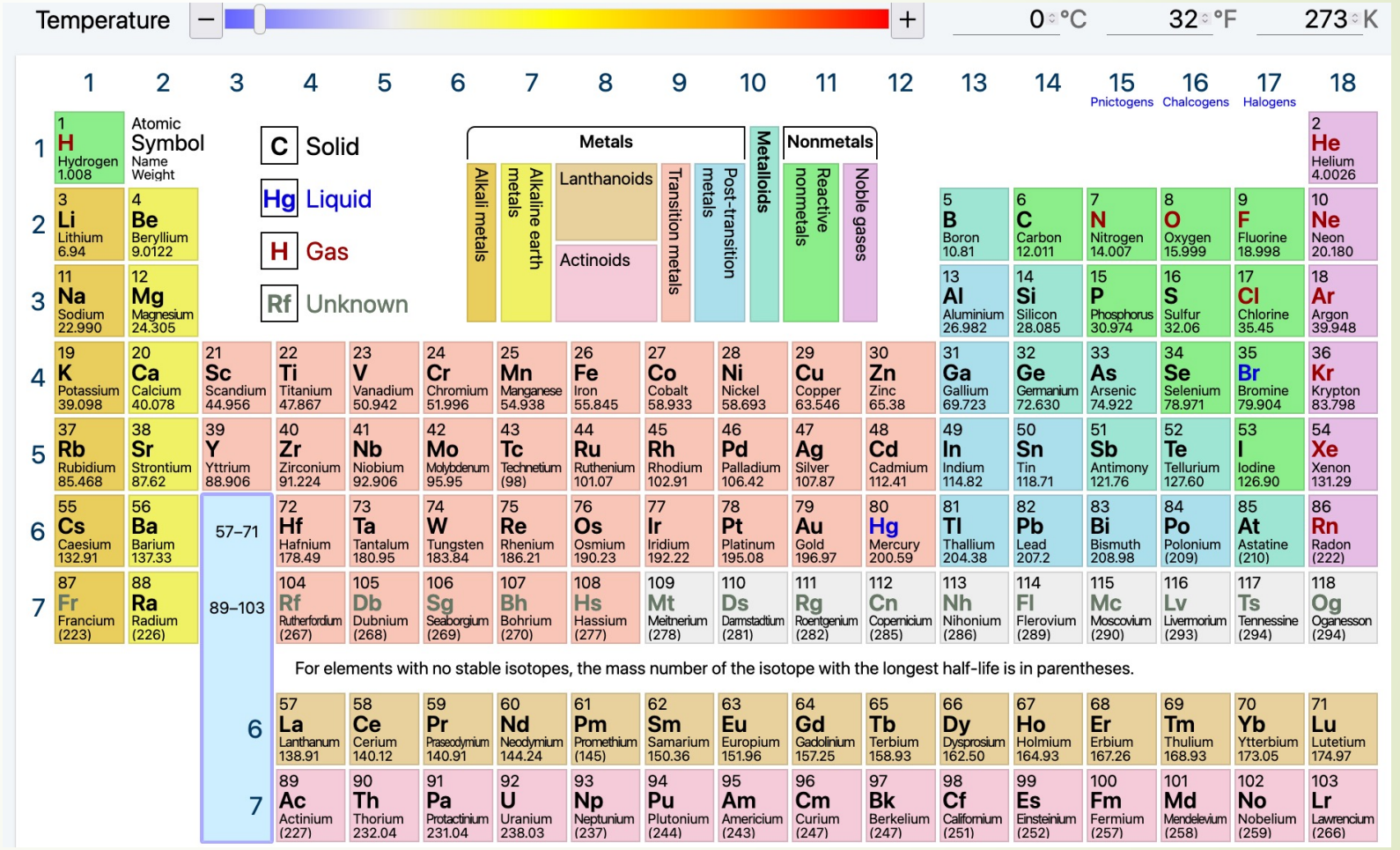
COMMON MATERIALS

- Periodic table lists all known 'elements'
- Elements form 'compounds'
- Example of Compound: H_2O

We drink water, breathe in O_2, exhale CO_2

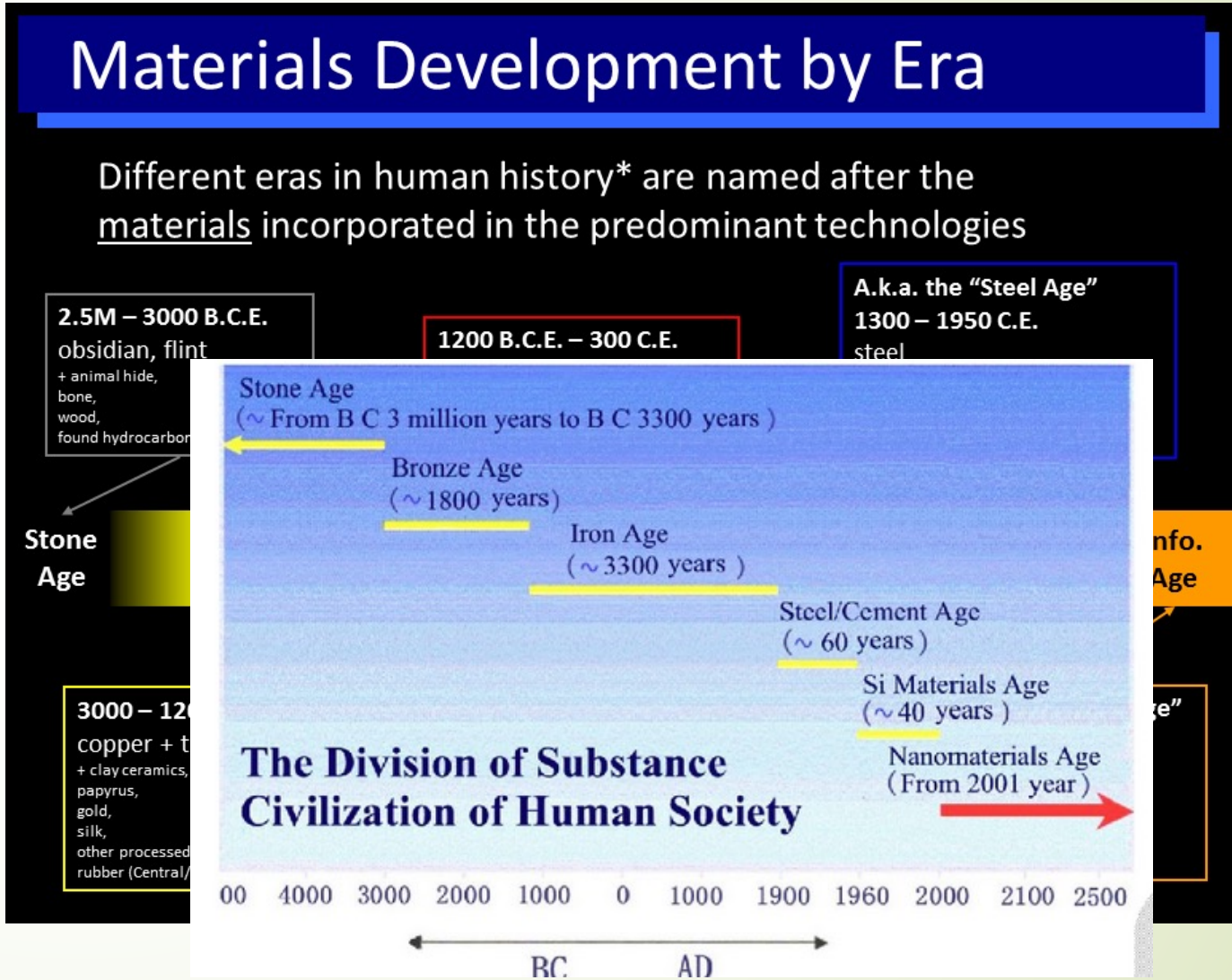
- We use materials for all our daily applications!!
  - Electric wires: metals
  - breakfast cereal: ceramic



PROGRESS OF OUR CIVILIZATION

https://www.cpp.edu/~jbputhoff/history.html

- Human progress has been determined by the development of materials
- The information age is driven by silicon
- Nanomaterials can impact all technology (more on this shortly)

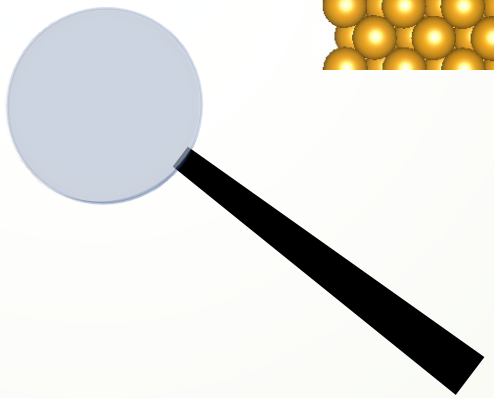


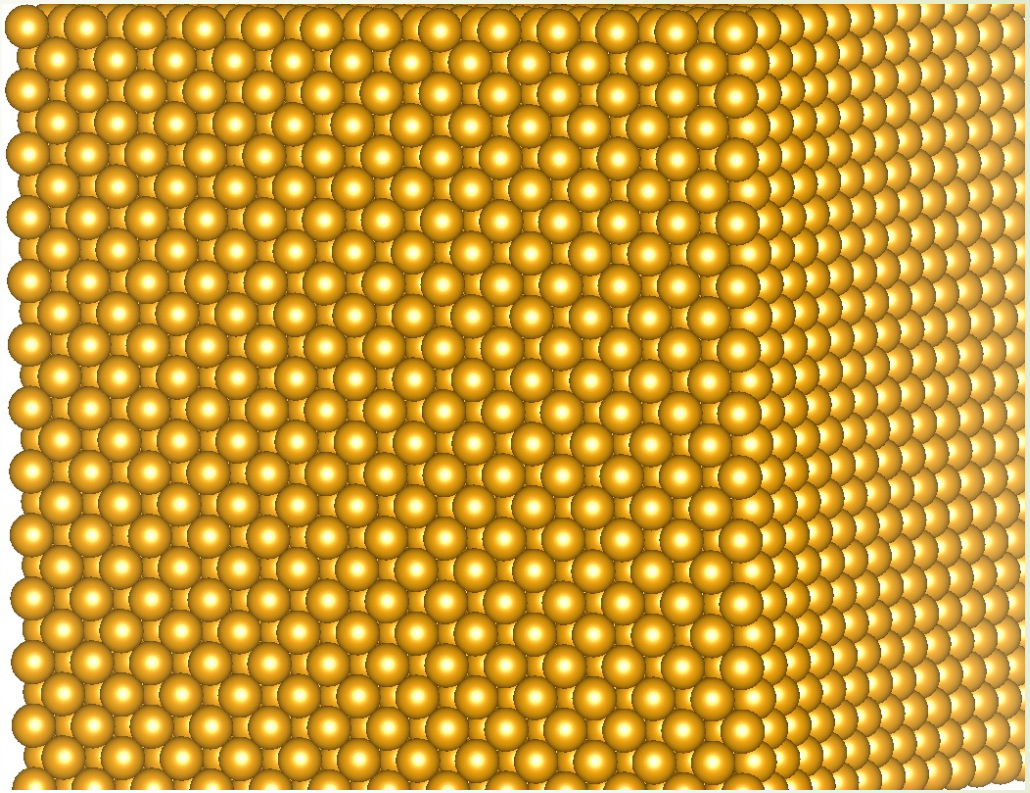
Bangwei, Z., *Arts and Social Sciences Journal* (2011)

GOLD

- Activity: Type the chemical symbol of Gold

Gold jewellery



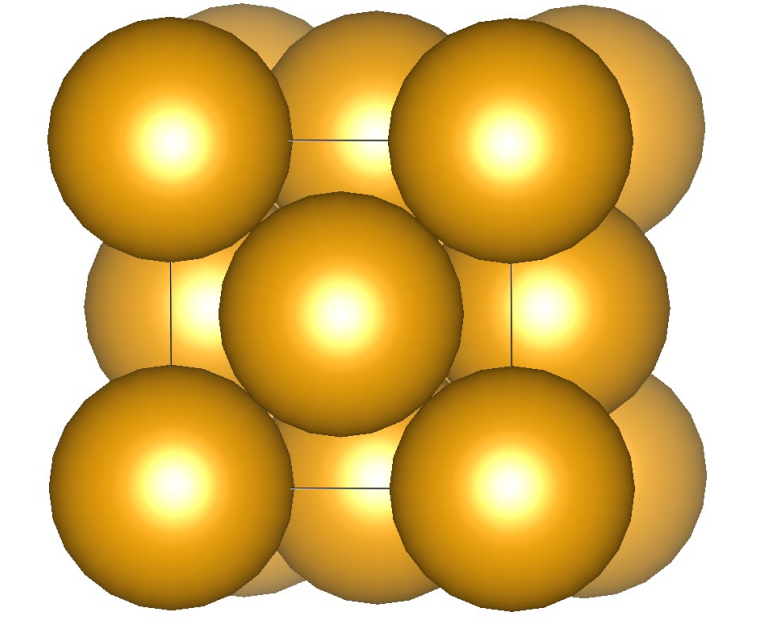


Gold Crystal

CRYSTAL STRUCTURE

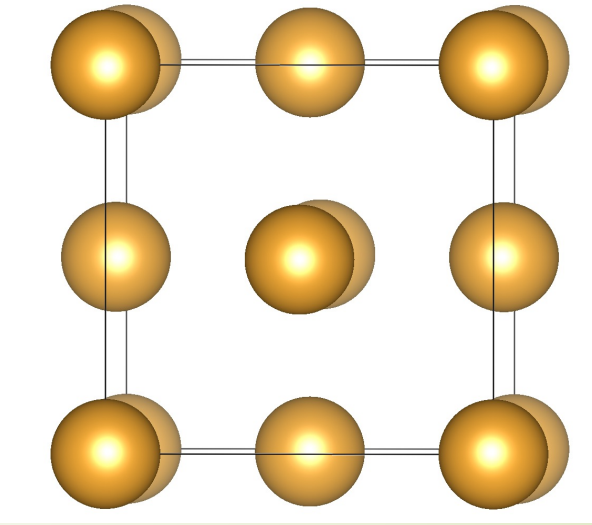
- Properties of Crystal:

1. three-dimensional (3D) repeating
2. ordered arrangement

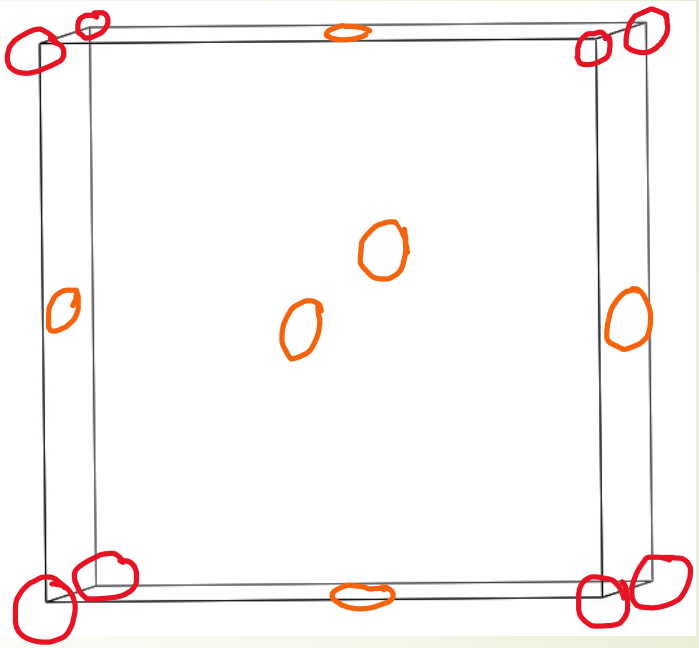


- How do we simplify this large structure?
- Unit-cell

-smallest repeating unit which gives us the crystal structure



Au CRYSTAL STRUCTURE



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- How do we simplify this large structure?
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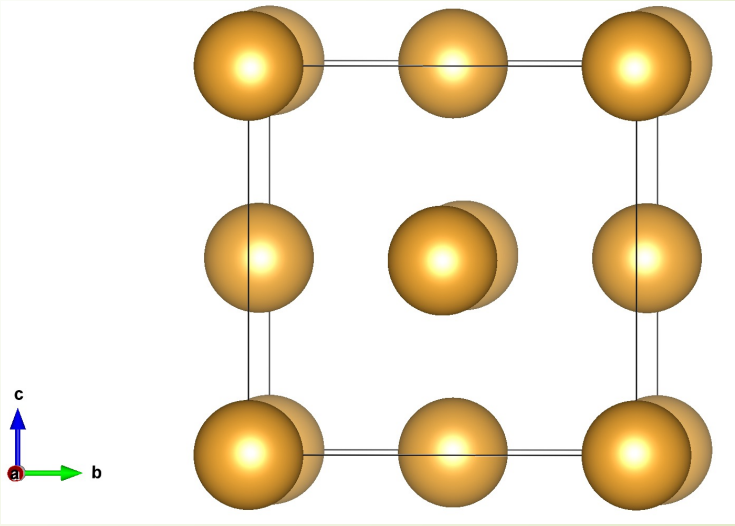
-smallest repeating unit which gives us the crystal structure

For gold, the structure is face-centered cubic (fcc)

- Atoms at corners of the cube
- Atoms at face-centers

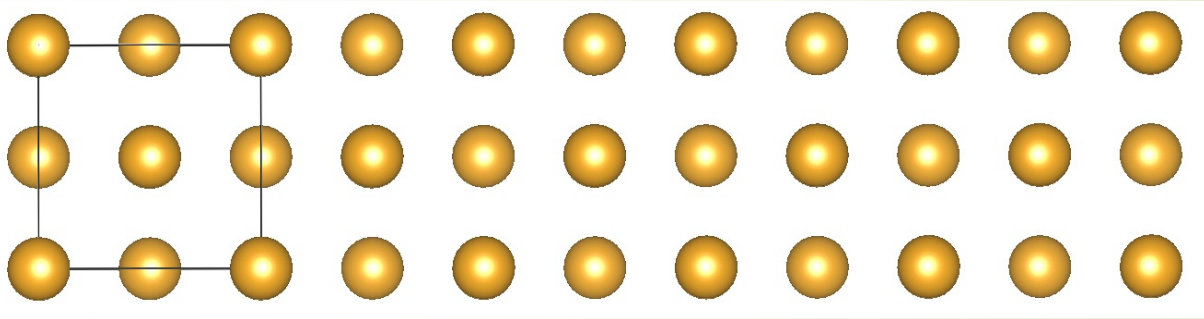
We will use VESTA to visualize the structures! (Hands-on)



LATTICE PARAMETER

- Lattice parameter (a) is an important characteristic of unit-cell

usually in Å units. 1 Å = 10^{-10} m



- For Au, a_Au = 4.08 Å

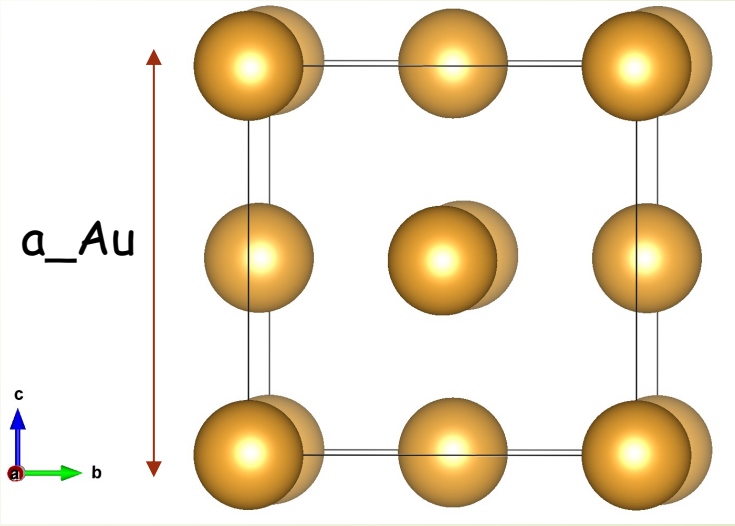
- QUIZ: What is the length of 5 unit-cells of Au?

A) 12.24 Å

B) 8.16 Å

C) 20.4 Å

D) 2.04 nm (nanometer, 10^{-9} m)



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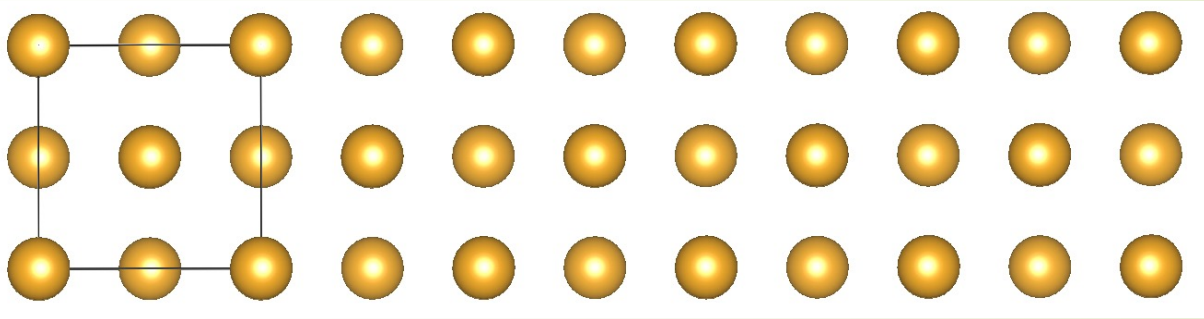

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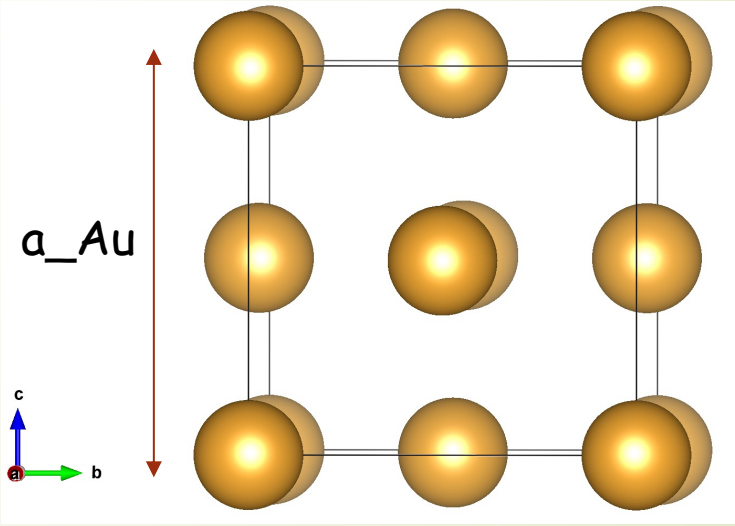
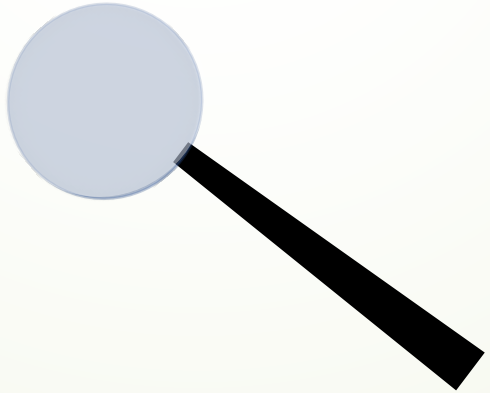
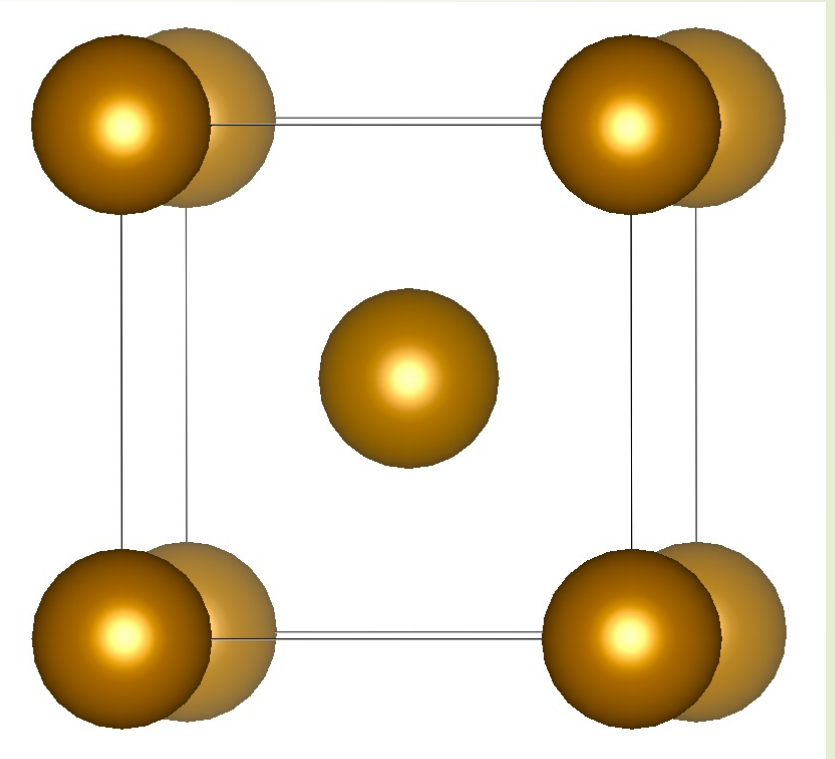


- Nanotechnology is the engineering of materials at nano scale!

Iron

- Activity: Type the chemical symbol of Iron

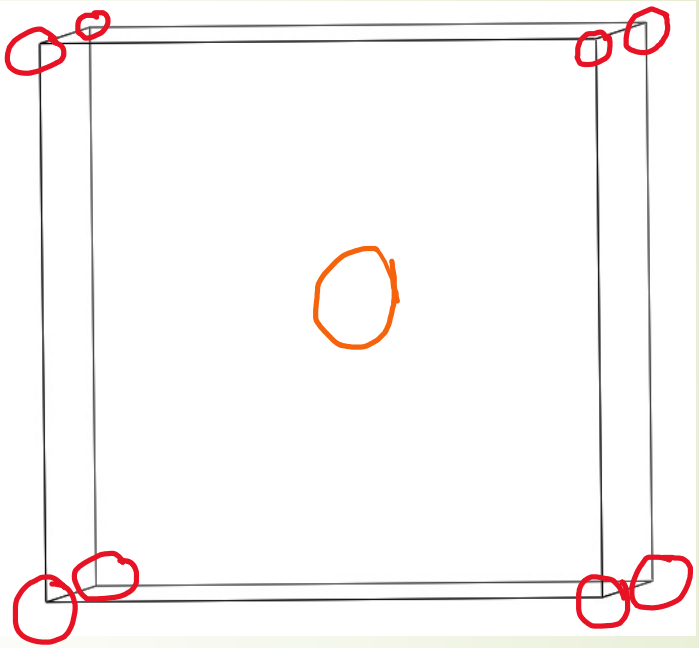




Fe CRYSTAL STRUCTURE

- For iron, the structure is body-centered cubic (bcc)

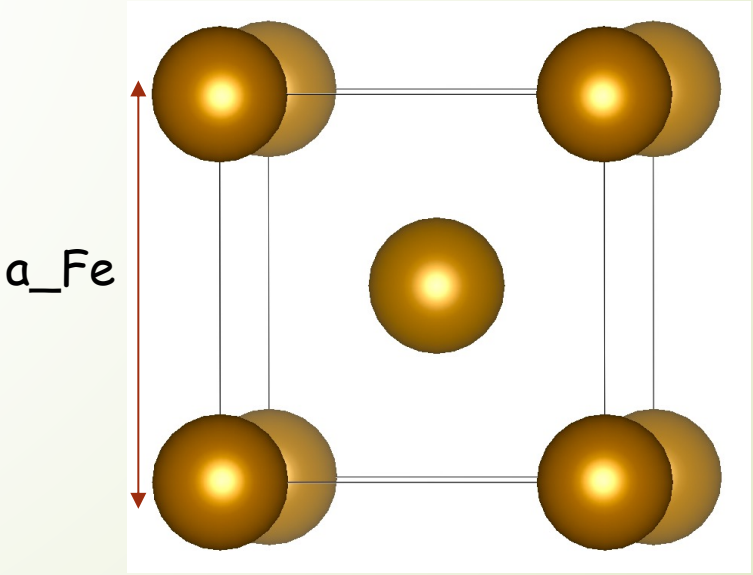
- Atoms at corners of the cube
- Atoms at center of the cube



- Lattice parameter (a)

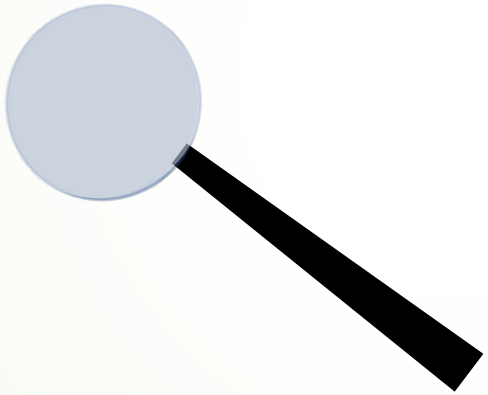
For Fe, a_Fe = 2.87 Å

We will use VESTA to visualize the structures! (Hands-on)

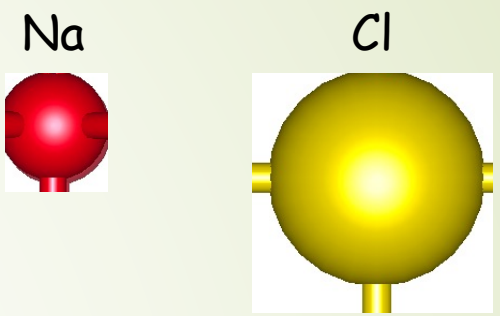


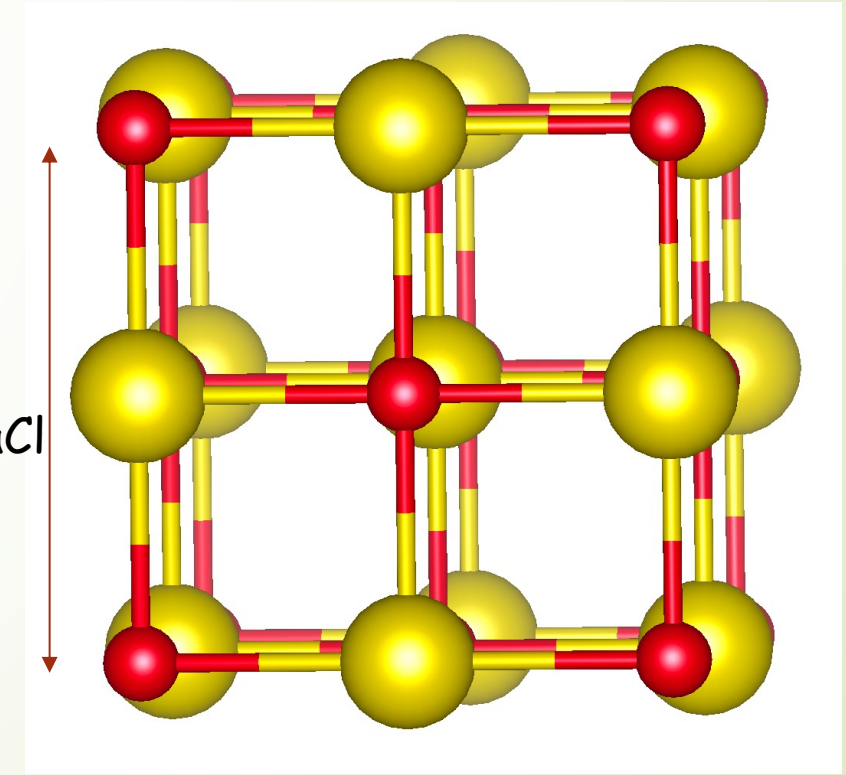
Common Salt

- Activity: What is the chemical formula of common salt?



- NaCl is a compound made of Na and Cl elements
- This structure is actually known as rocksalt structure
- Lattice parameter (a), a_NaCl = 5.64 Å





NEAREST-NEIGHBORS

- The closest neighbor of an atom is its 'nearest-neighbor'
- Let us consider this one face of a gold (Au) unit-cell
- Quiz: What is the value of d-1NN in terms of a?

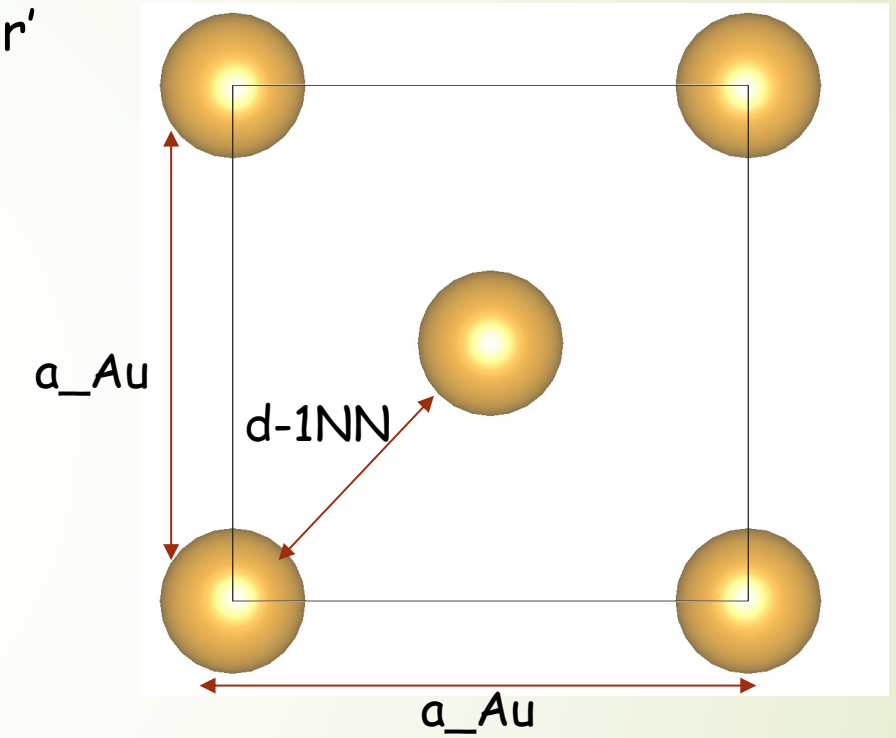
(Hint: face of a cube is a square)

A) a/2

B) $a/\sqrt{2}$

C) $a\sqrt{2}$

D) a/4



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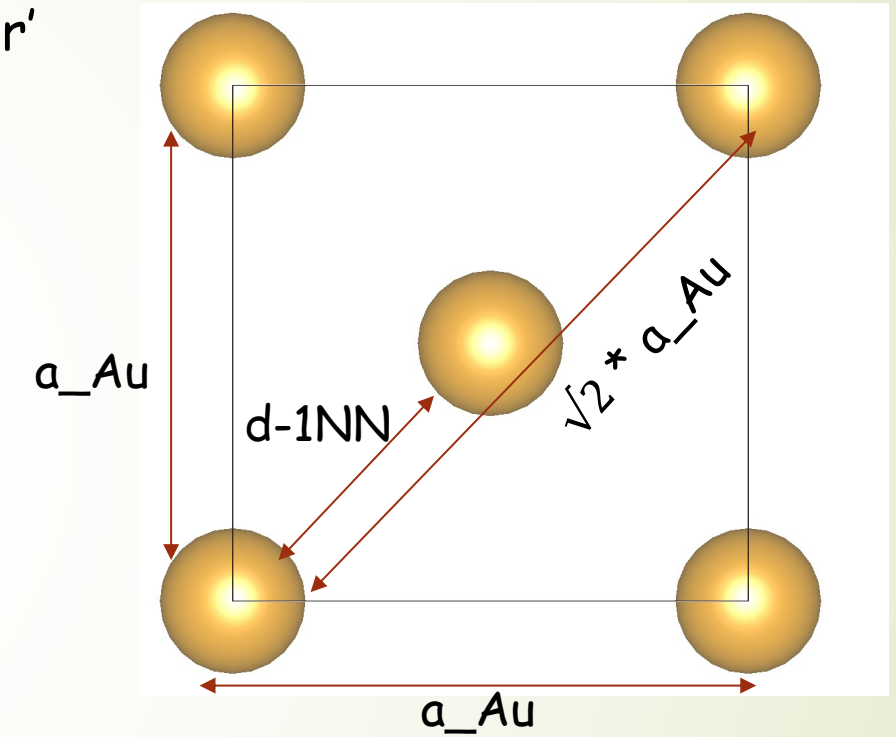
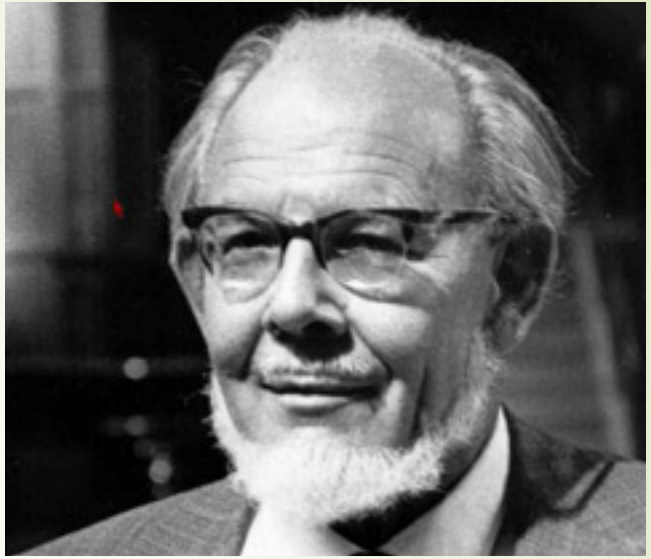


- Similarly, second nearest-neighbor is d-2NN away, which is …

a (lattice constant)

- Volume of unit-cell = a^3 (volume of cube)

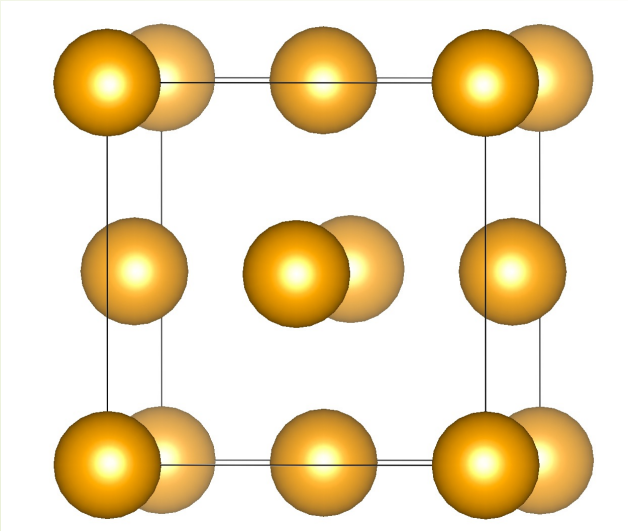
DEFECTS

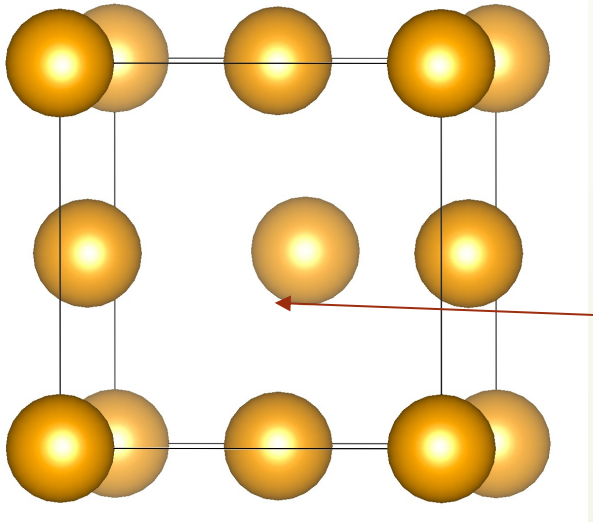


- The atoms do not always sit in their usual positions -> Defects
- Defects are common in materials and impact the properties

"Crystals are like people: it is the defects in them that make them interesting." Charles Frank

- Materials Science and Engineering aims to engineer new materials
- Goal is to understand defects and how they impact material properties



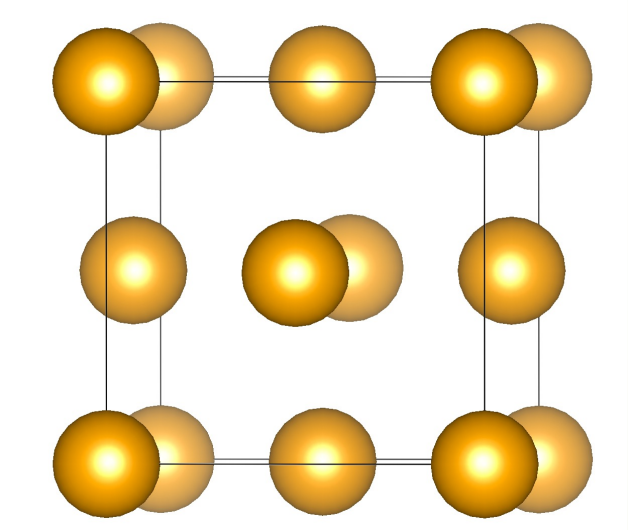


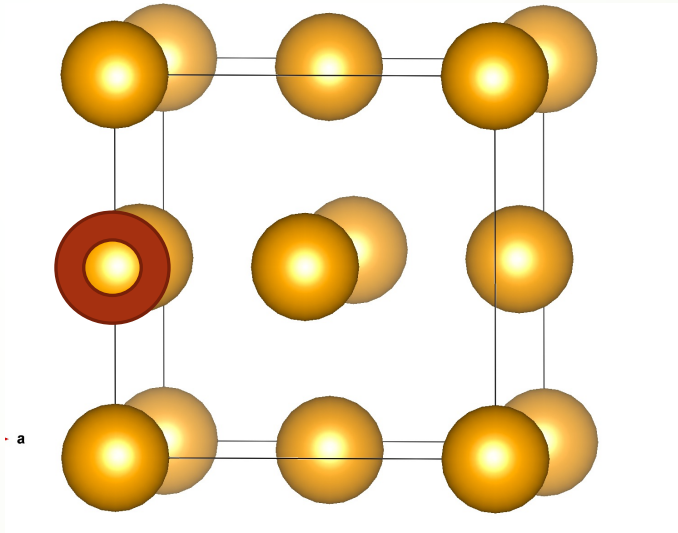
DEFECTS IN MATERIALS

- Types of defects:

a) vacancies: atom missing from its usual site

b) interstitials: atom at an interstitial (void between atoms) site





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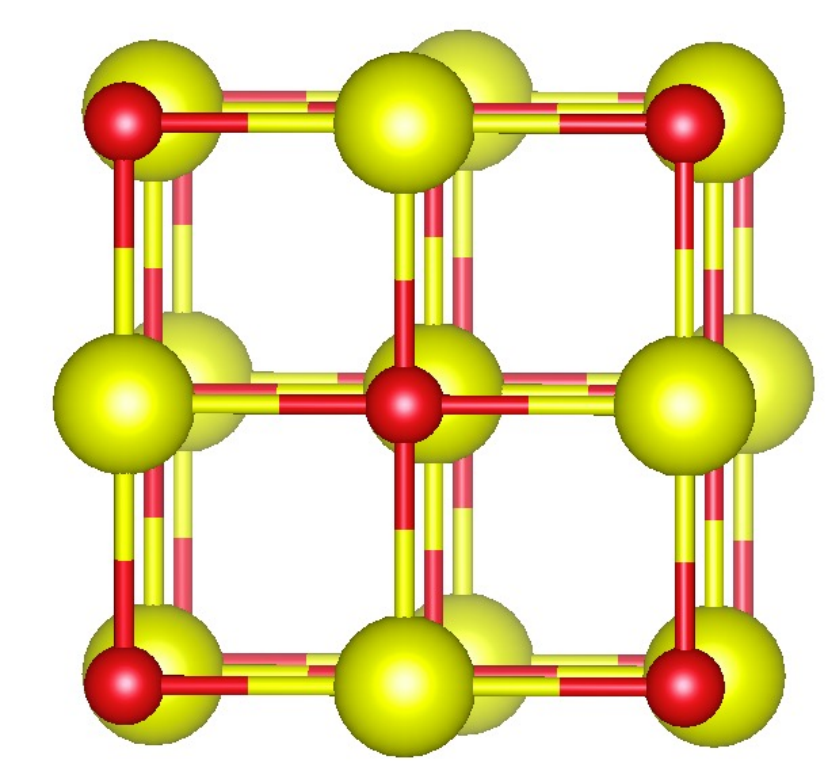

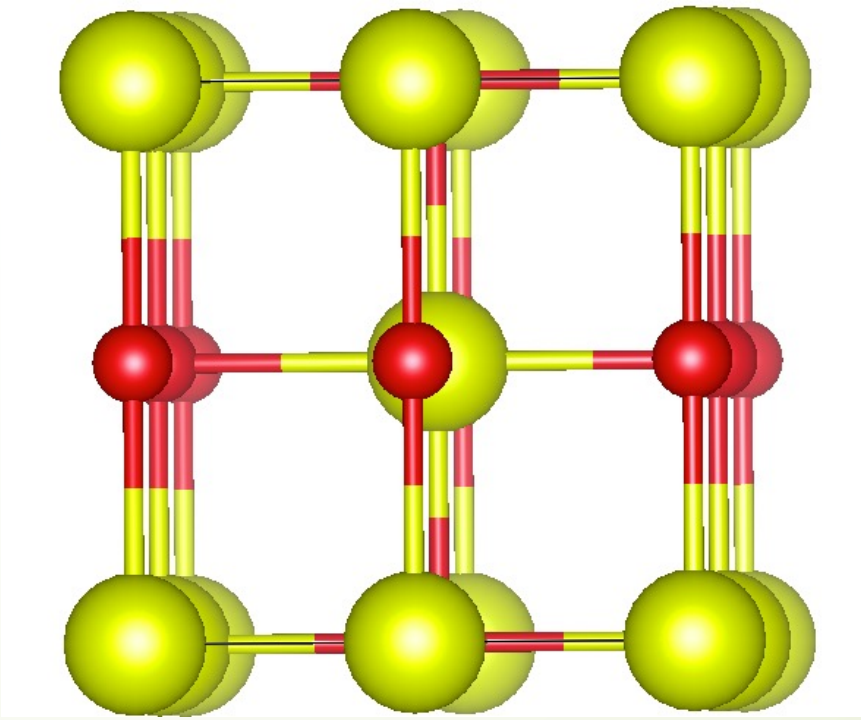

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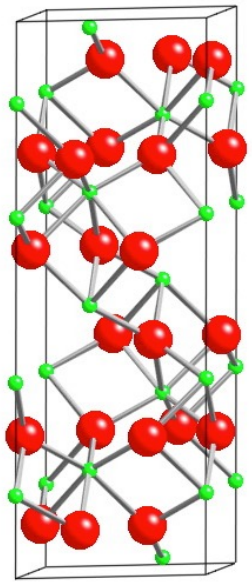
- Above defects are intrinsic, often we introduce defects externally these are called extrinsic defects
- Si is extrinsically doped to increase the number of charge carriers!

color due to Ti and Fe



pure Al_2O_3 (transparent)

color due to Cr defects

KEY POINTS

- Materials are everywhere around us, their development is linked to our progress
- We represent a crystal structure using its unit-cell with a lattice parameter.
- Defects in materials can be of intrinsic as well as extrinsic type.
- Defects can play a key role to tune the desired properties of materials.
- Materials Science and Engineering aims to understand materials at a fundamental level and try to design new ones by engineering defects in the material.

RESOURCES

- https://youtu.be/dLPgqobwPGE
- https://steemit.com/life/@zest/the-three-age-system-the-stone-age-the-bronze-age-and-the-iron-age
- https://en.wikipedia.org/wiki/History_of_materials_science
- https://www.doitpoms.ac.uk/tlplib/crystallography3/unit_cell.php
- https://www.nano.gov/timeline
- self-healing material (slightly older video) https://youtu.be/kX_kiECXkvM