MAT SCI 104 Winter 2025:
Science of Engineering Materials

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Department of Materials Science & Engineering

What is a “material” exactly?



Steel

Plastics



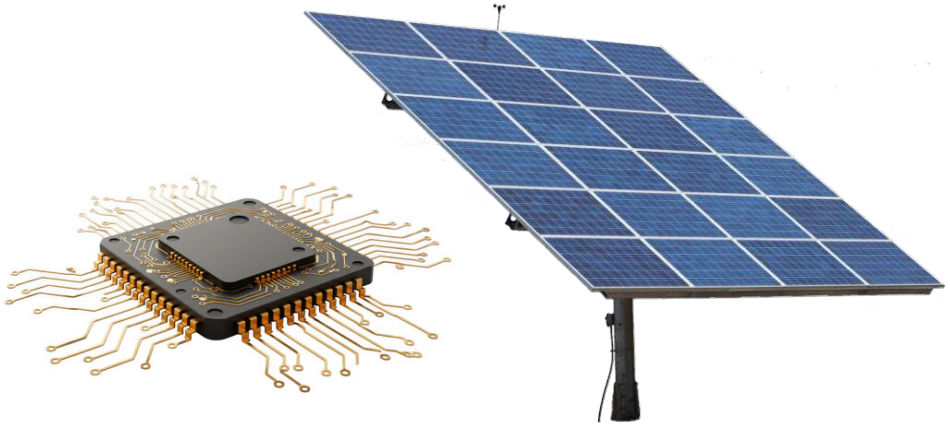


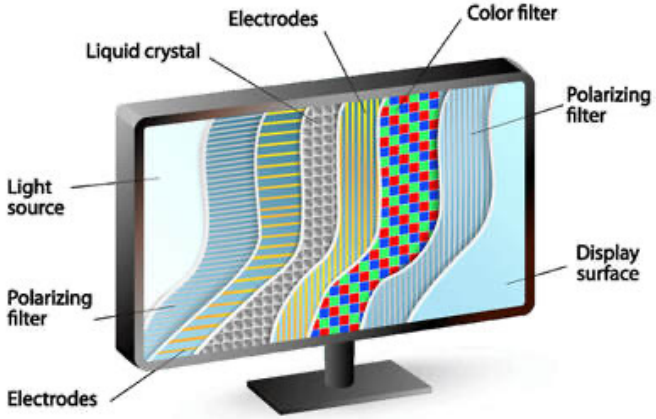
Glass

Cement



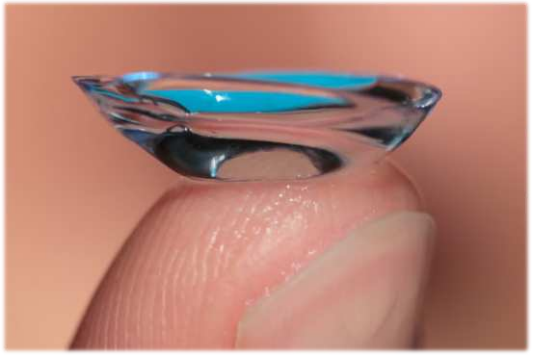
Semiconductors





Liquid crystals

Hydrogels



Materials have defined ages in history



Stone Age
(→ 3300 BC)









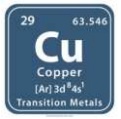


Iron Age
(1200 → 500 BC)

Then?



Bronze Age
(3300 → 1200 BC)















Materials have defined ages in history



Industrial Age (1750 → 1900)







Semiconductors (1950 → 2000)

? ?







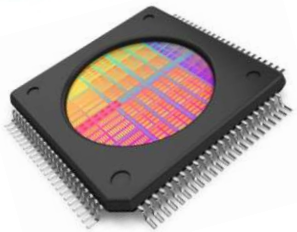
Modern Materials (1900 → 1950)





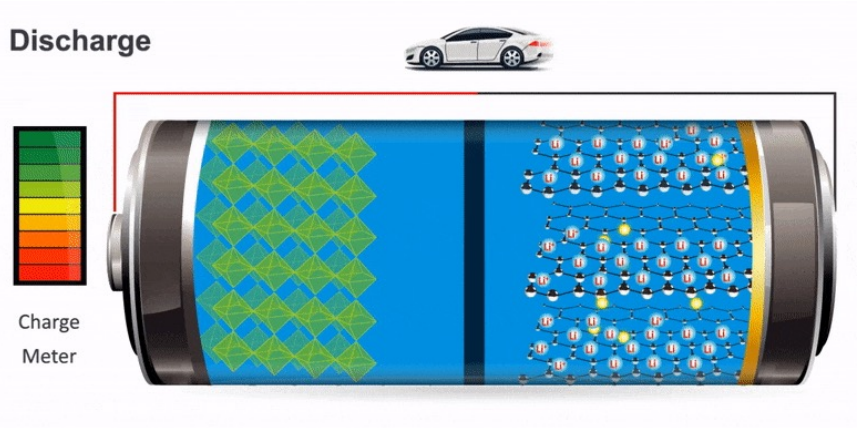
Advanced Materials (2000 →)







We are in the age of “advanced” materials

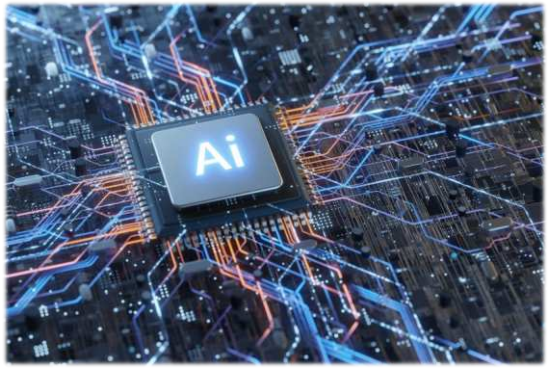


Lithium-ion batteries

Superalloys

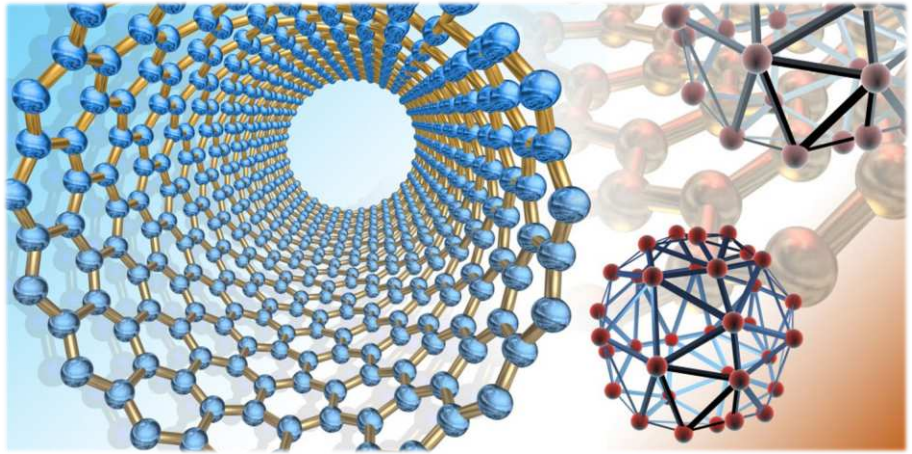


Chips for AI



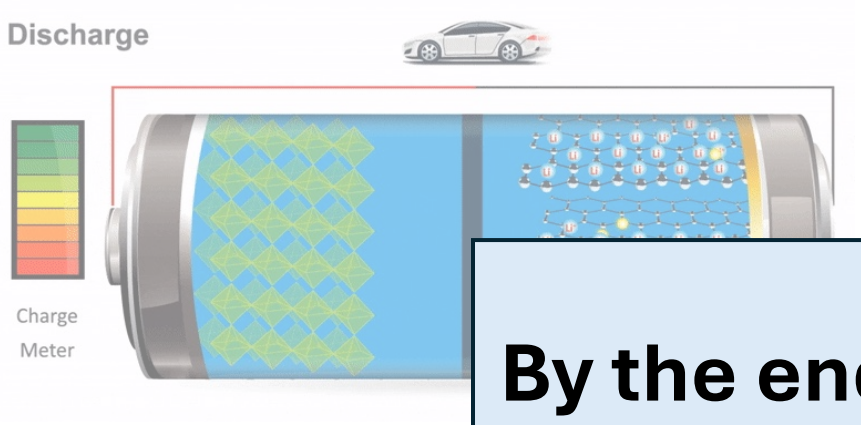


Shape memory alloys



Nano and quantum materials

We are in the age of “advanced” materials



Lithium-ion batt

Superalloys



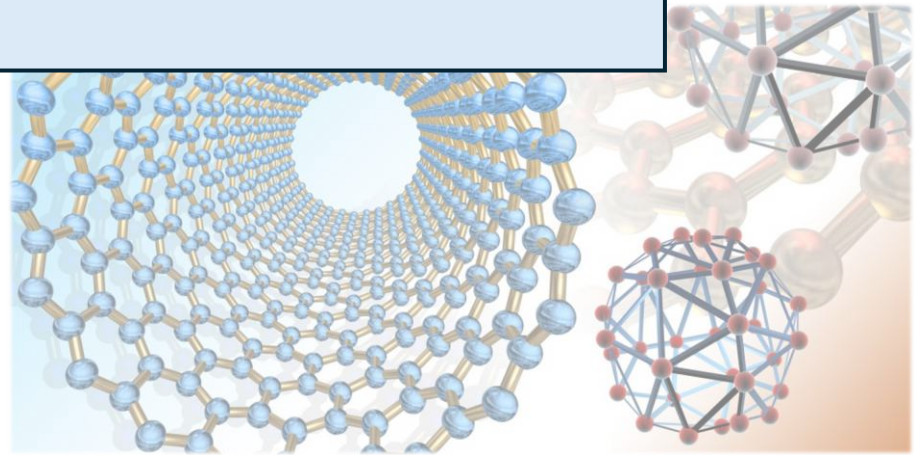
Chips for AI



By the end of this course: you should know how to *design* materials for these applications



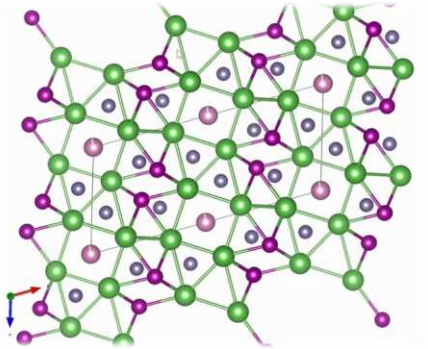
Shape memory alloys



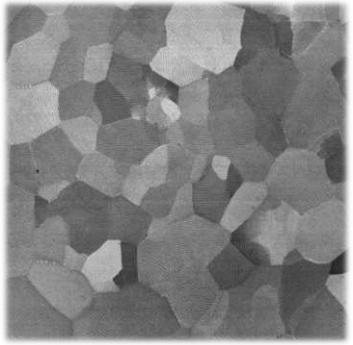
Nano and quantum materials

What is there to know about materials?

Structure



Atomic scale



Microscale

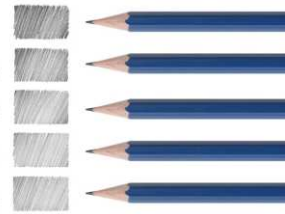
What is there to know about materials?





Carbon





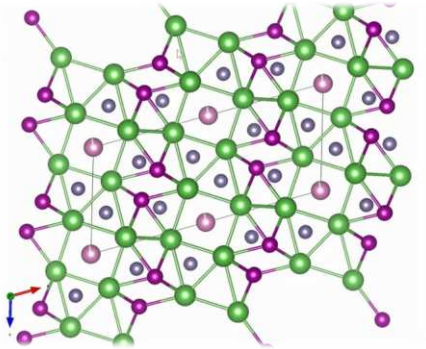




Diamond

Graphite

Structure



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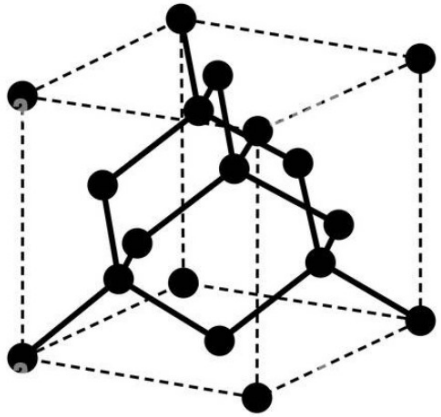
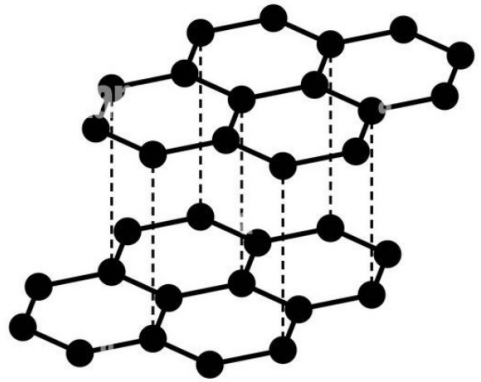
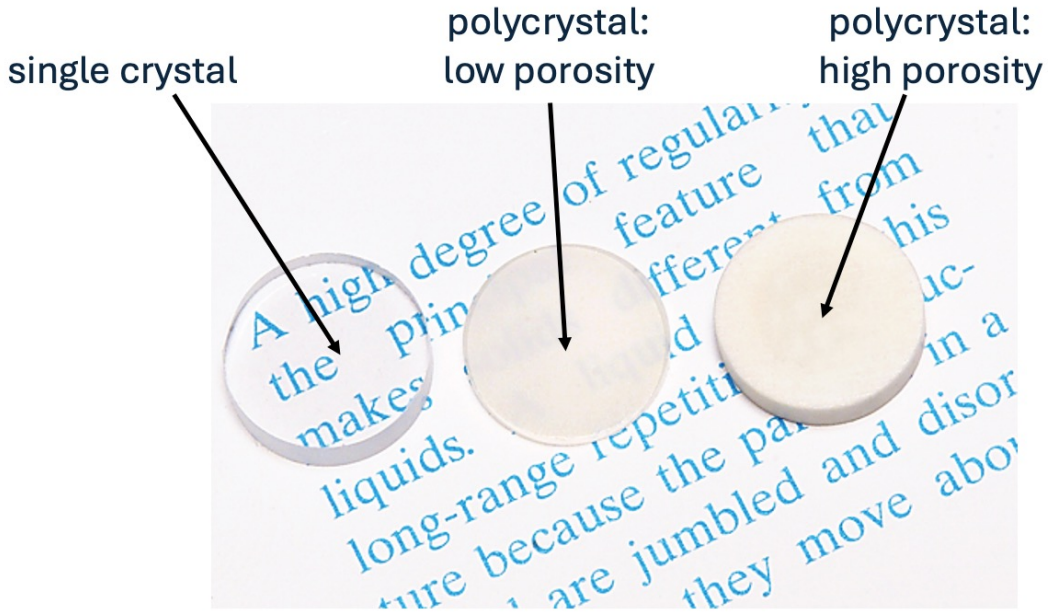






What is there to know about materials?



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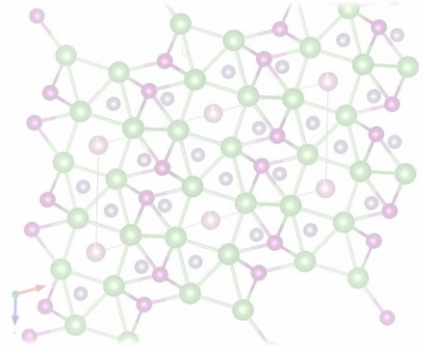
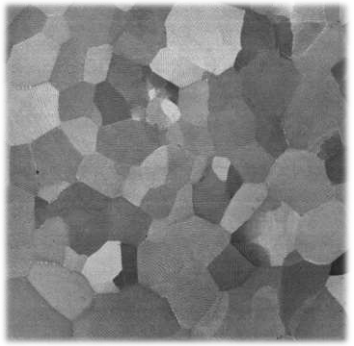
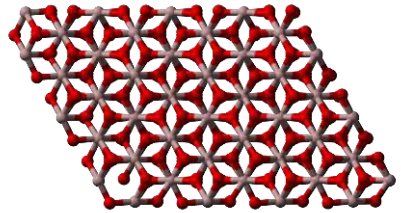


Atomic scale

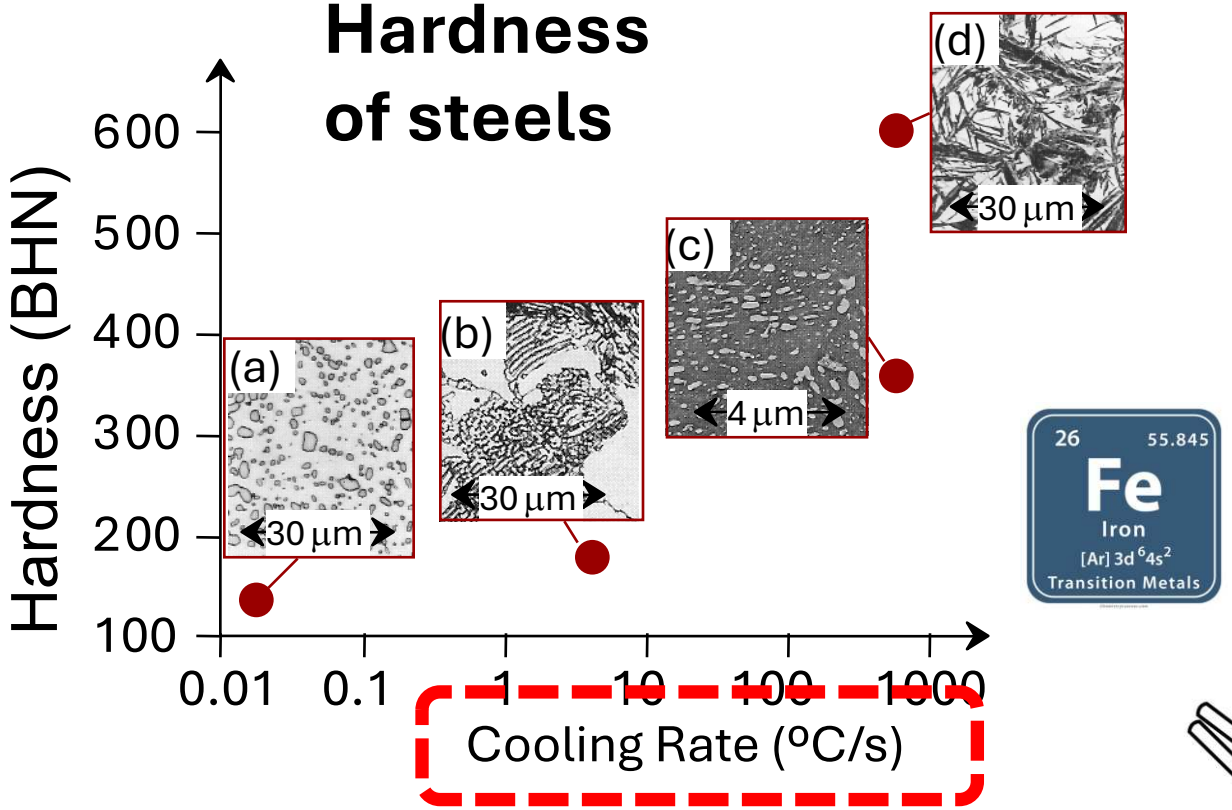


Microscale

Optical transparency of alumina (Al_2O_3)



Hardness of steels



What is there to know about materials?

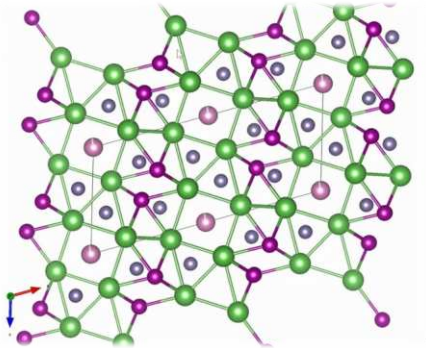
Synthesis & Processing



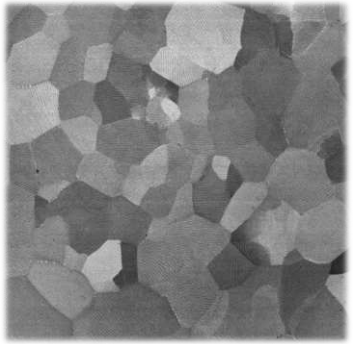


Is controlled by...

Structure



Atomic scale



Microscale

What is there to know about materials?

Synthesis & Processing





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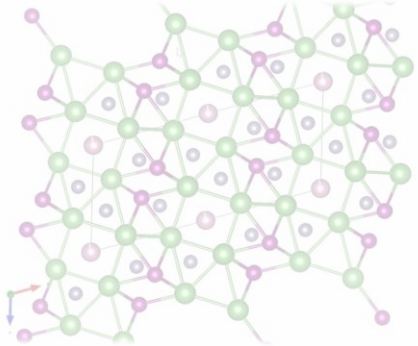
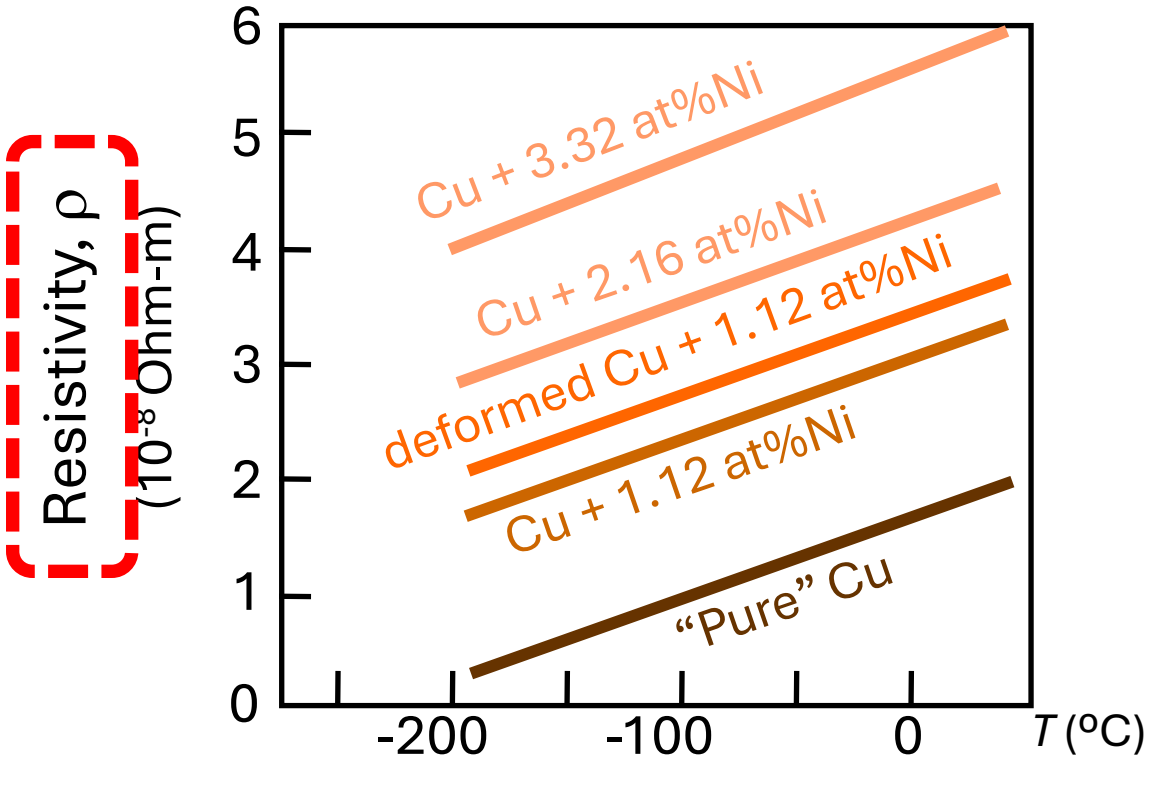
Structure



Atomic scale

Microscale



What is there to know about materials?

Synthesis & Processing





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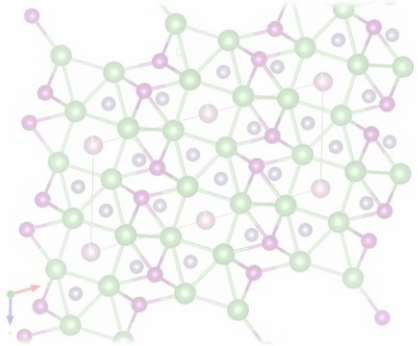
Dictates...

Structure



Atomic scale

Microscale

Properties



What is there to know about materials?

Synthesis & Processing





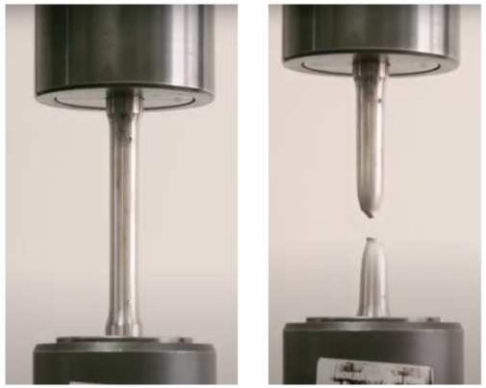
Is controlled by...

Dictates...

Structure

Properties

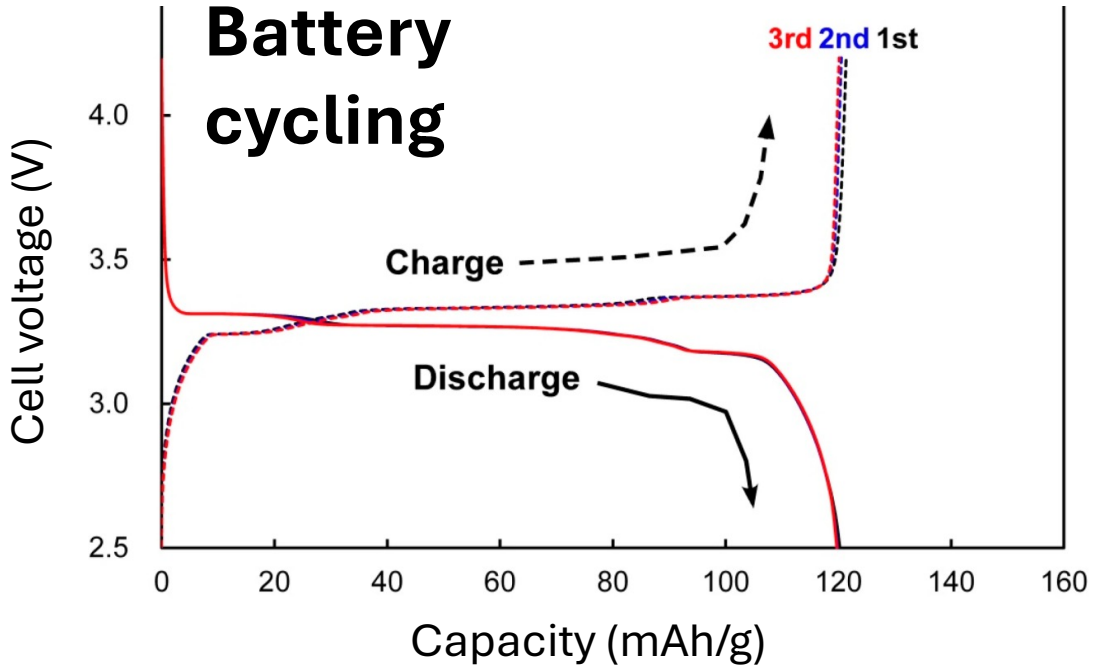




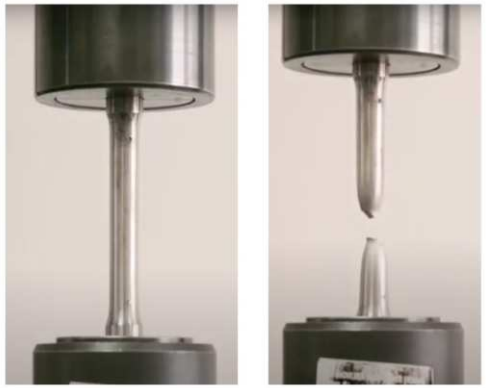
Governs...

Performance

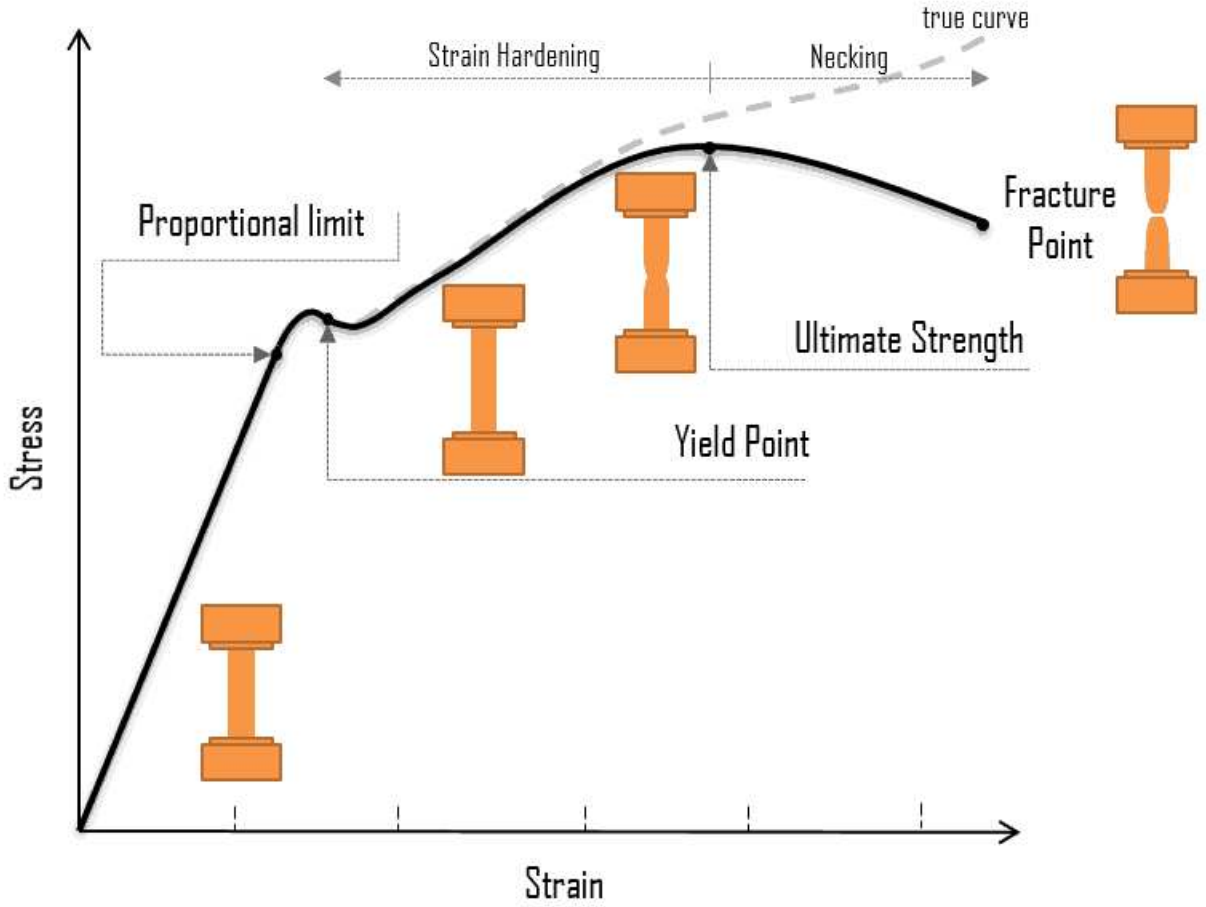
What is there to know about materials?







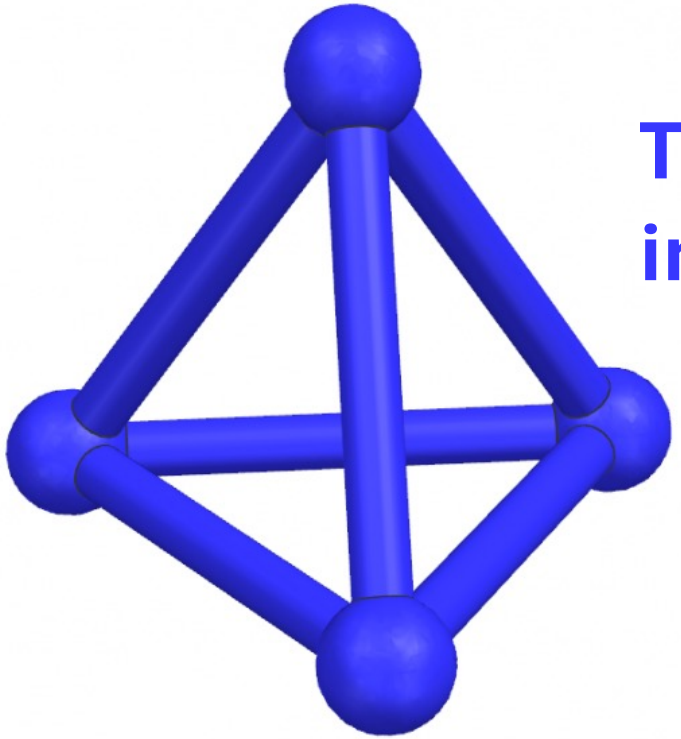
Mechanical testing



What is there to know about materials?

The materials tetrahedron

Synthesis & Processing



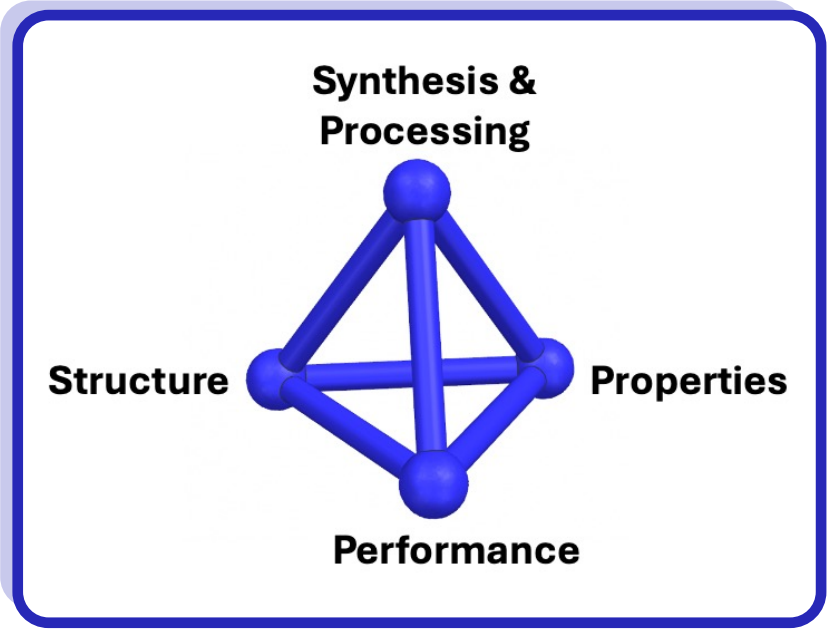
Structure

Properties

Performance

These are all interconnected!

Materials are often categorized by structure, properties, application, *etc.*



Metals

- Very dense structure
- Moderate T_m
- Conductive
- Strong/ductile

Ceramics

- Less dense structure
- Very high T_m
- Insulating
- Hard but fragile

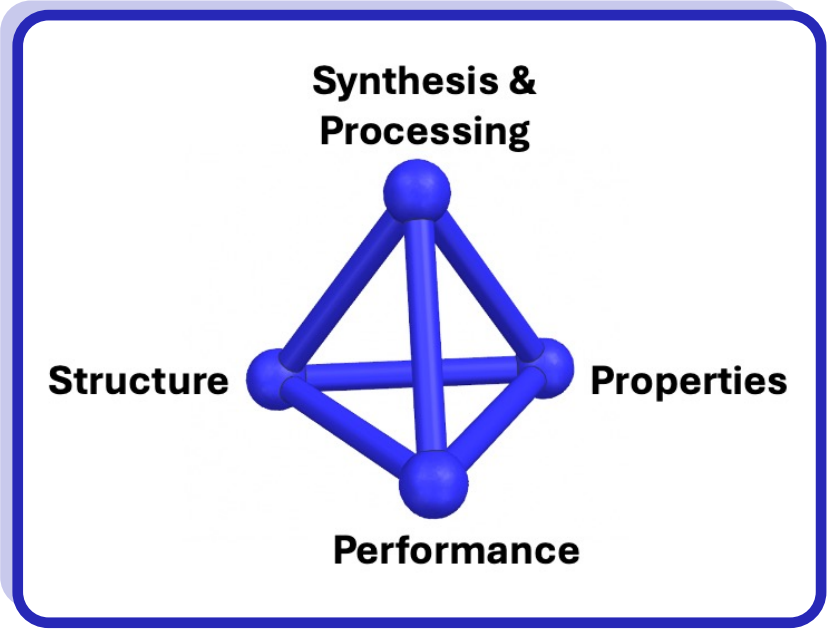
Semiconductors

- "In between" metals and ceramics
- Moderate strength, conductivity, *etc.*

Polymers

- Very low density
- Usually low T_m
- Insulating
- Often very soft and ductile, "stretchable"

Materials are often categorized by structure, properties, application, *etc.*



Composites

Combinations of these material types

Metals

- Very dense structure
- Moderate T_m
- Conductive
- Strong/ductile

Ceramics

- Less dense structure
- Very high T_m
- Insulating
- Hard but fragile

Semiconductors

- "In between" metals and ceramics
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Polymers

- Very low density
- Usually low T_m
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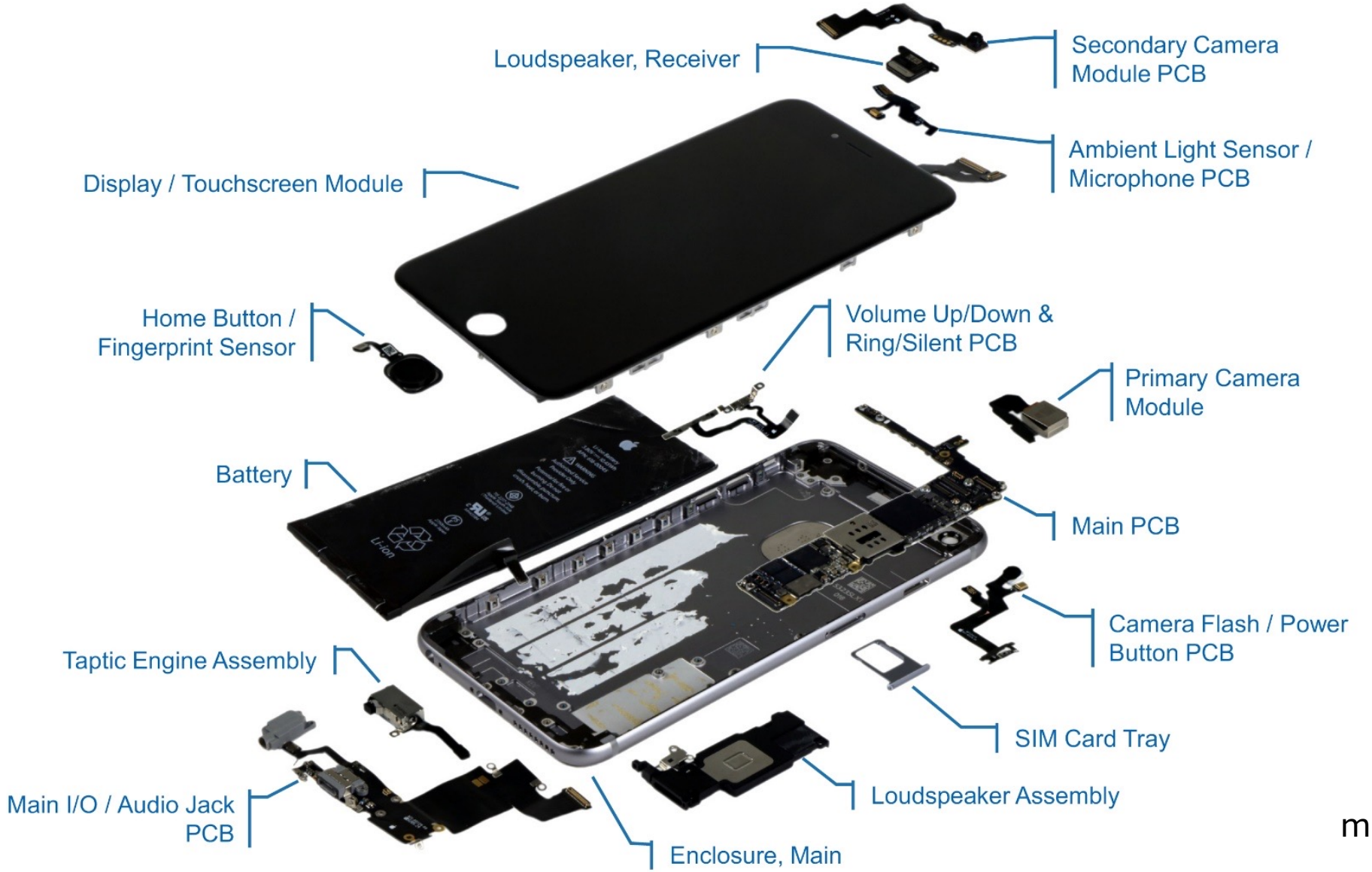
Many technologies use all different types!



TCO screens,
Li-ion batteries,
piezoelectrics,
metal/plastic casing,
and many more...

There are so many options…How do we know when to use each type of material?

Usually we “work our way backwards” – ***inverse design***



There are so many options…How do we know when to use each type of material?

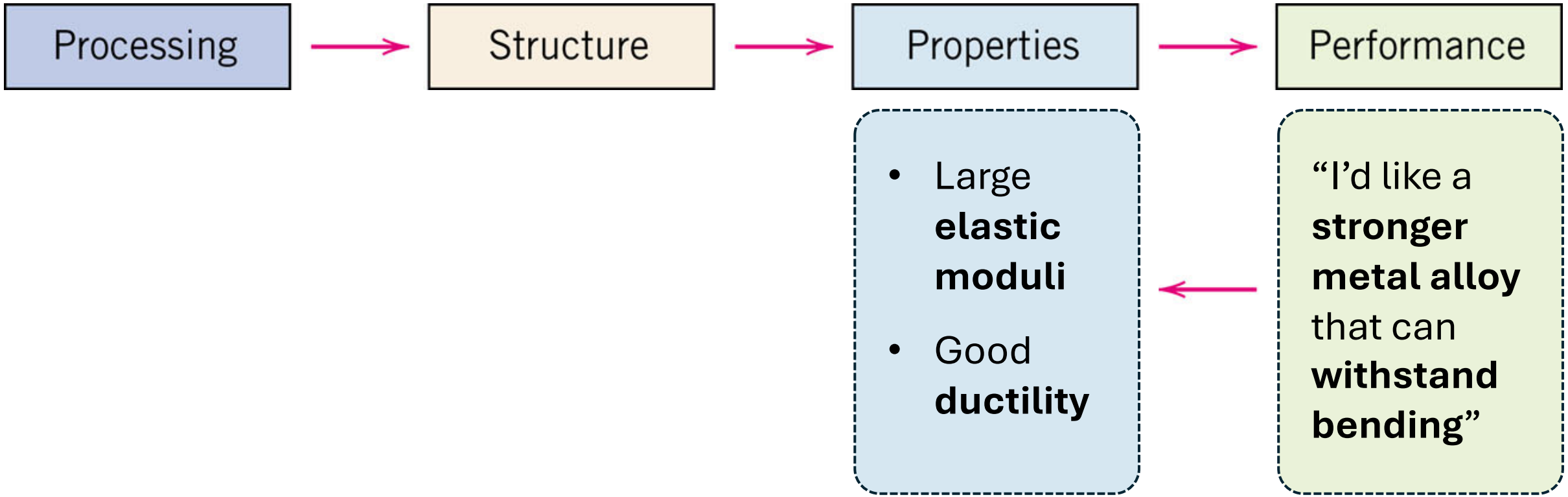
Usually we "work our way backwards" – ***inverse design***



"I'd like a **stronger metal alloy** that can **withstand bending**"

There are so many options…How do we know when to use each type of material?

Usually we "work our way backwards" – ***inverse design***



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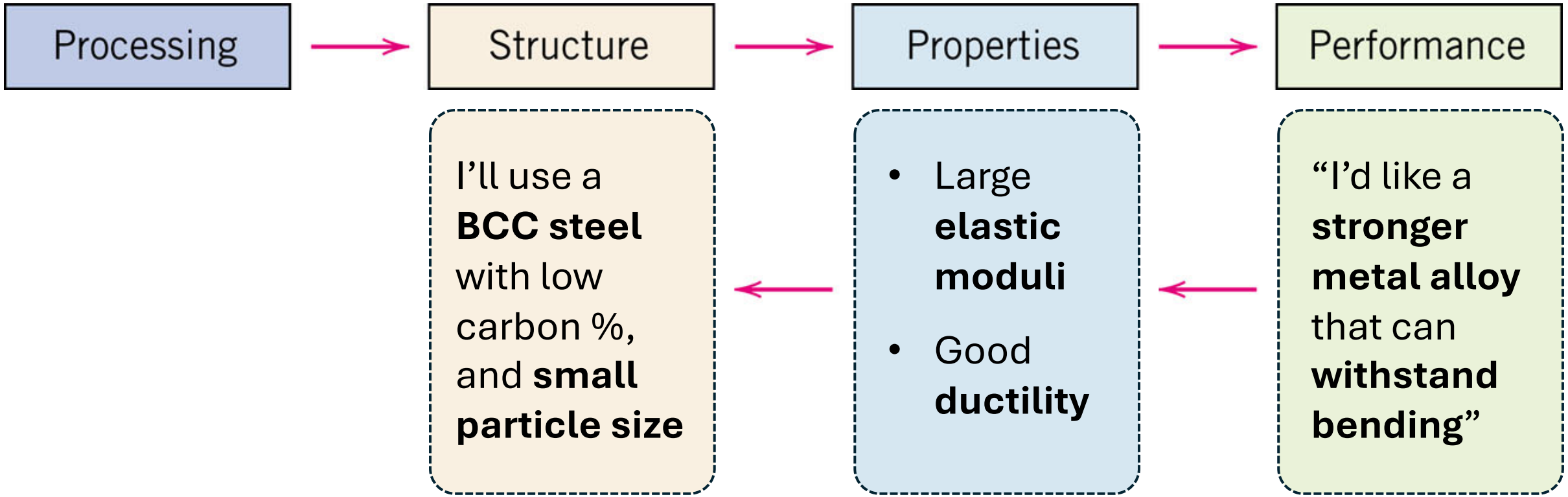

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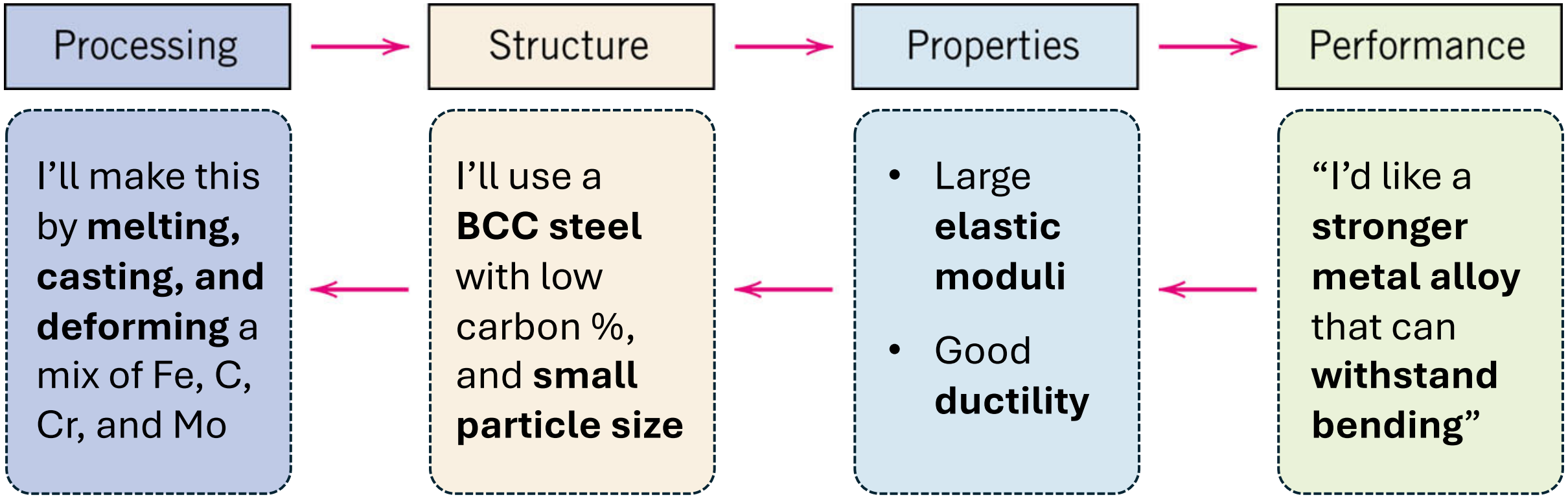
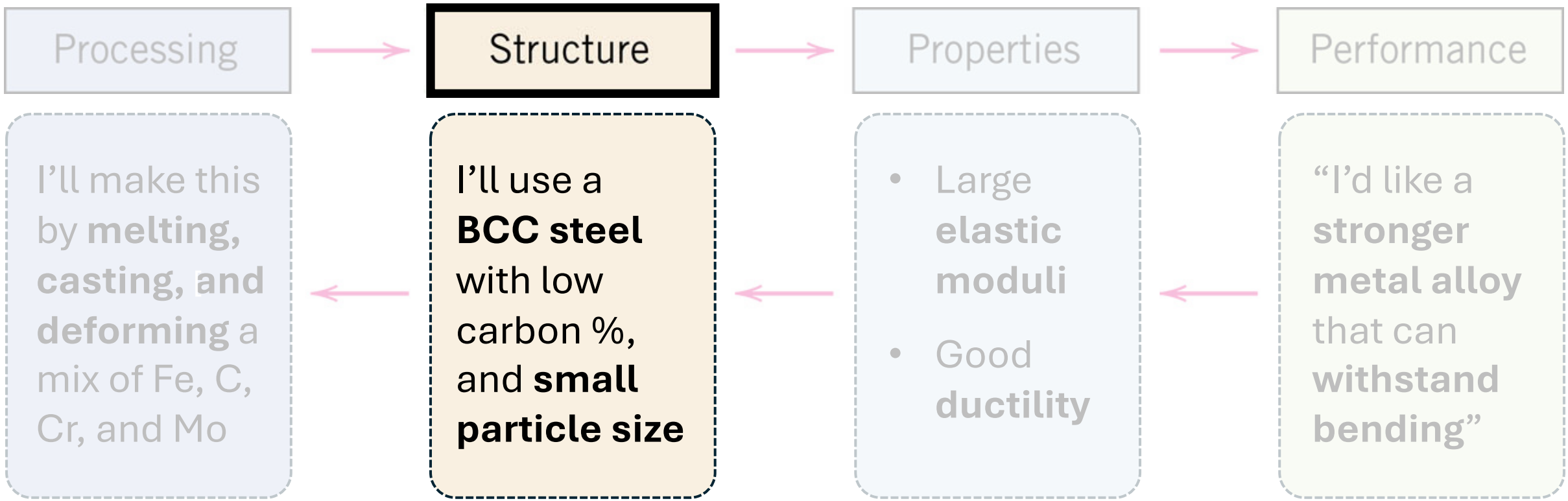
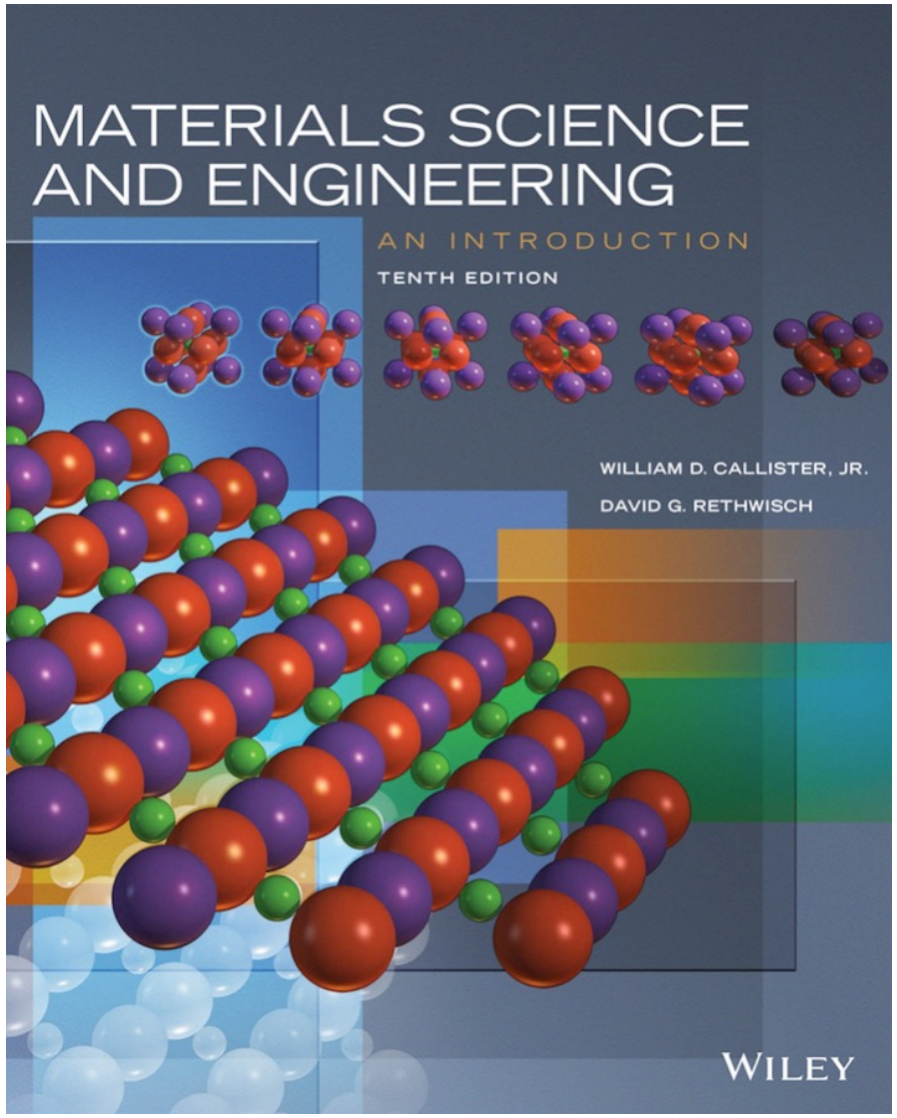


There are so many options…How do we know when to use each type of material?

Structure is arguably the most fundamental – let's start here



Atomic Structure and Interatomic Bonding



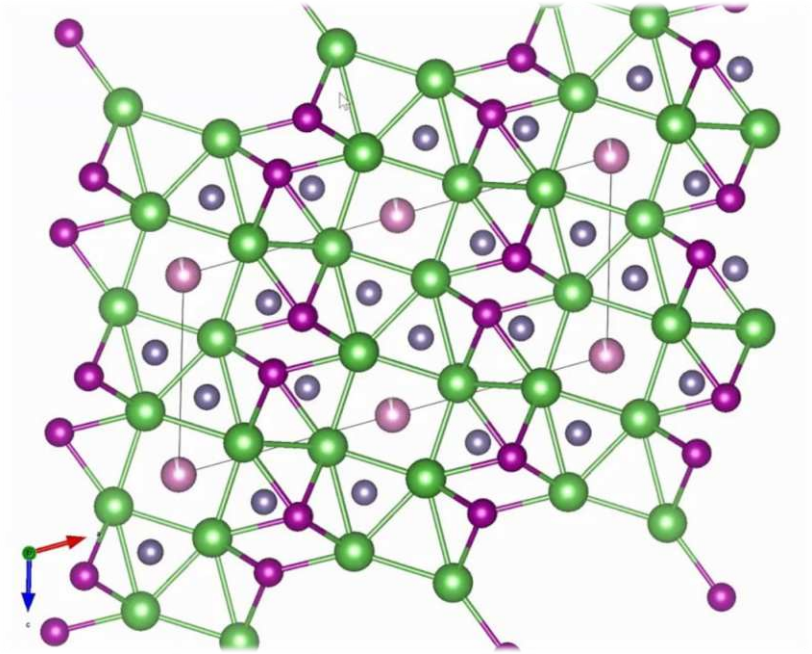
Chapter 2 Atomic Structure and Interatomic Bonding

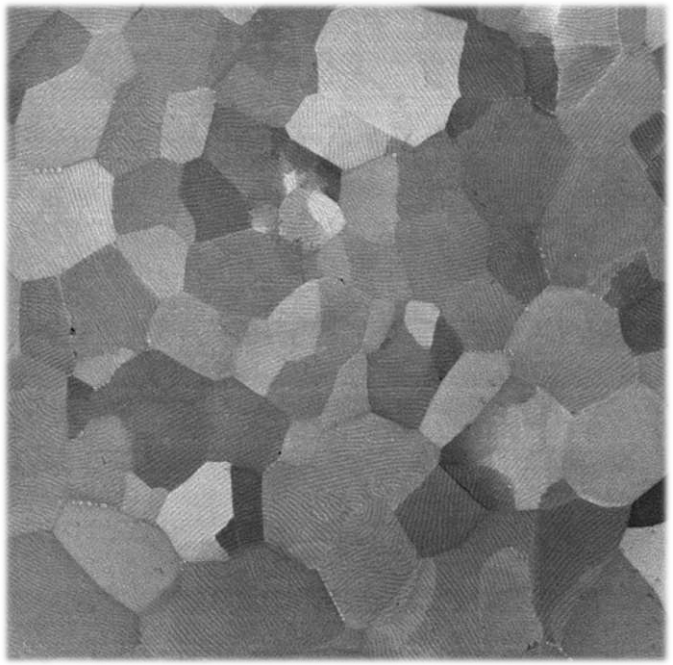
This discussion will closely follow **Chapter 2** of Callister, **pages 20-47** of the 10th edition. please take some time and read it! Our exams/quizzes will often pull from this book

Supplementary Texts:

- *Chemical Structure and Bonding* by DeCock
- *Solid-State Materials Chemistry* by Woodward
- *Ceramic Materials* by Carter

Atomic Structure and Interatomic Bonding



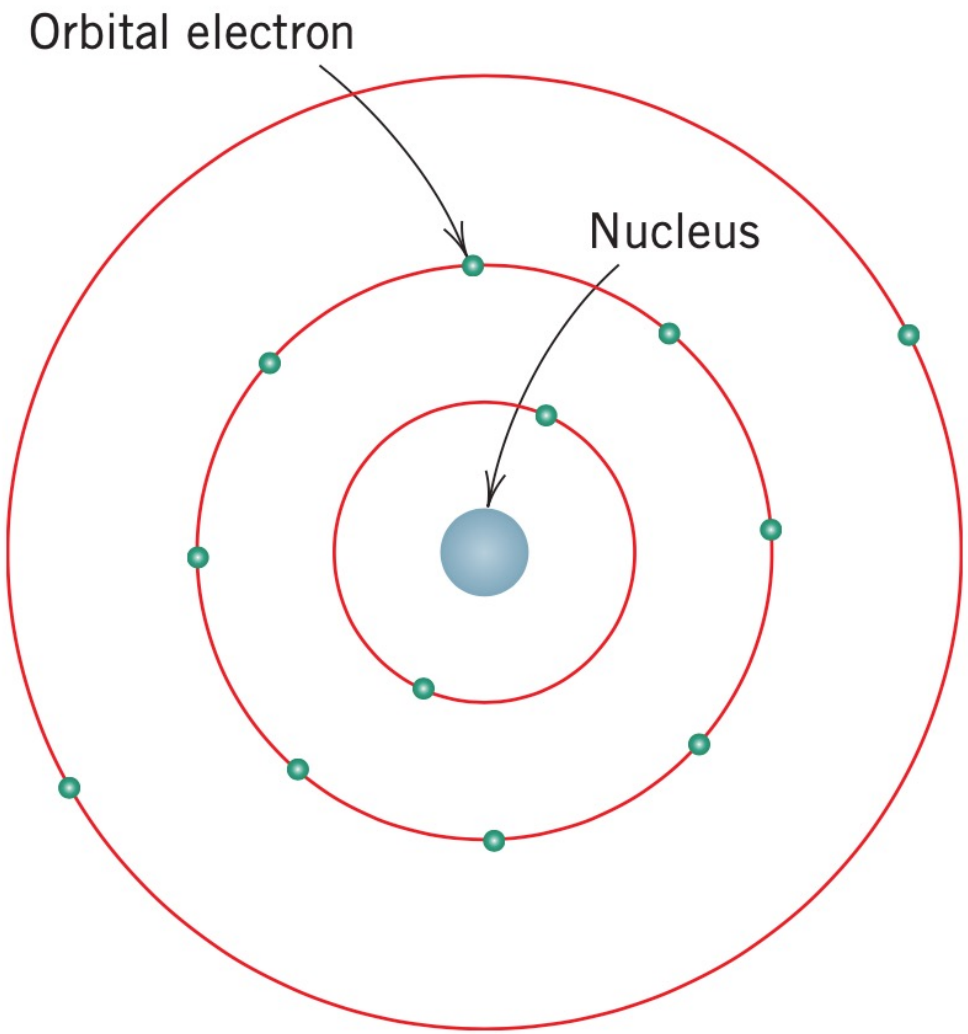




Before we talk about “structure” as a whole, we need to zoom in…

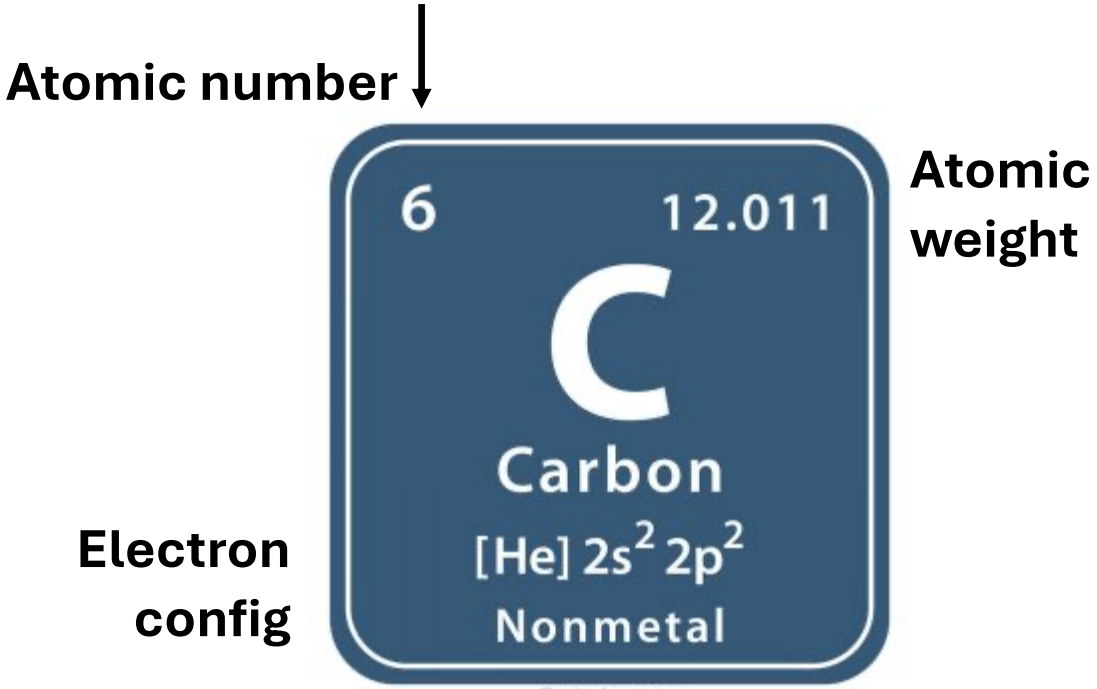
What is it about the ***atoms*** themselves that makes them want to bond in the first place?

A single atom = nucleus + electrons



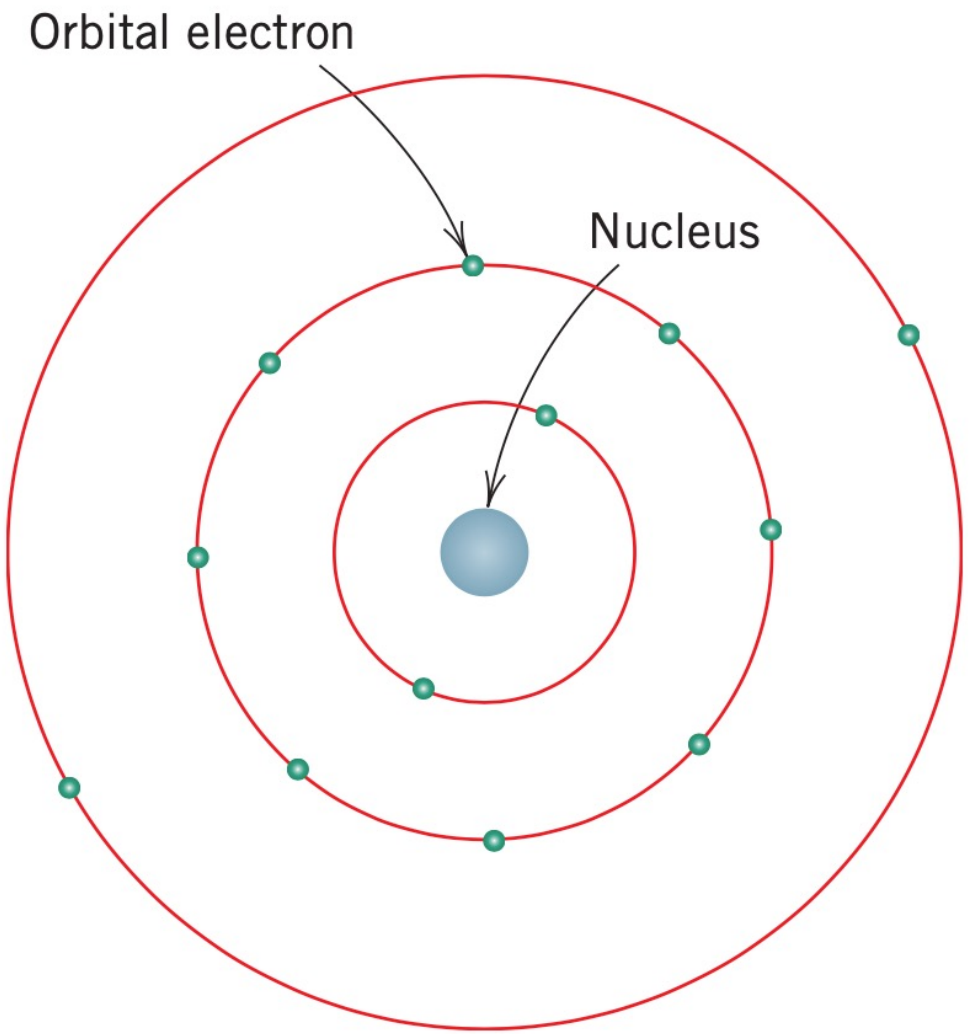
^Classical picture of the atom (Bohr model)

- Nucleus = **protons** + neutrons



- **Electrons** orbit around the nucleus, or more precisely: **occupy orbitals**

Electrons occupy orbitals in *discrete* energy levels



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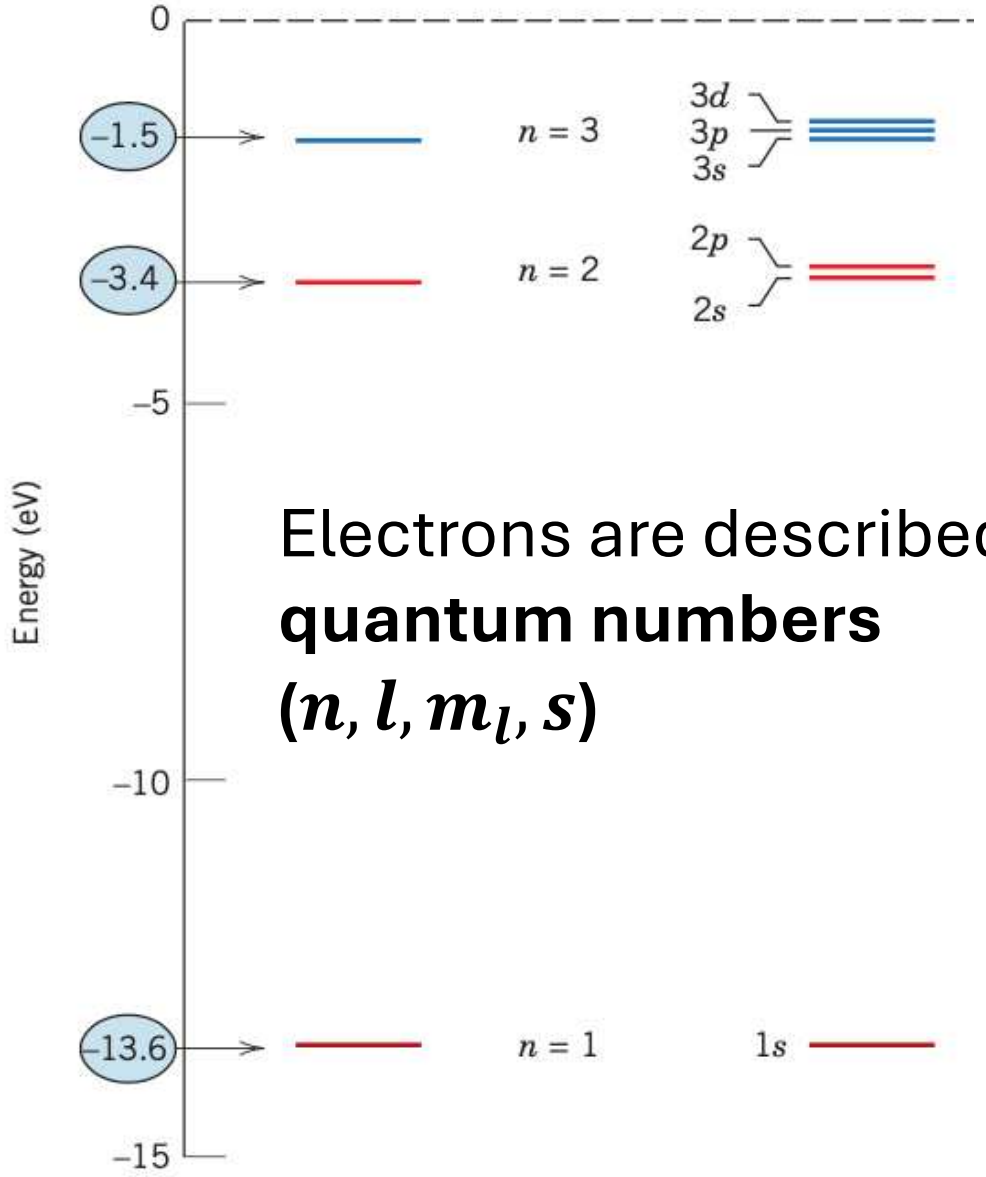


Electrons are described by **quantum numbers** (n, l, m_l, s)

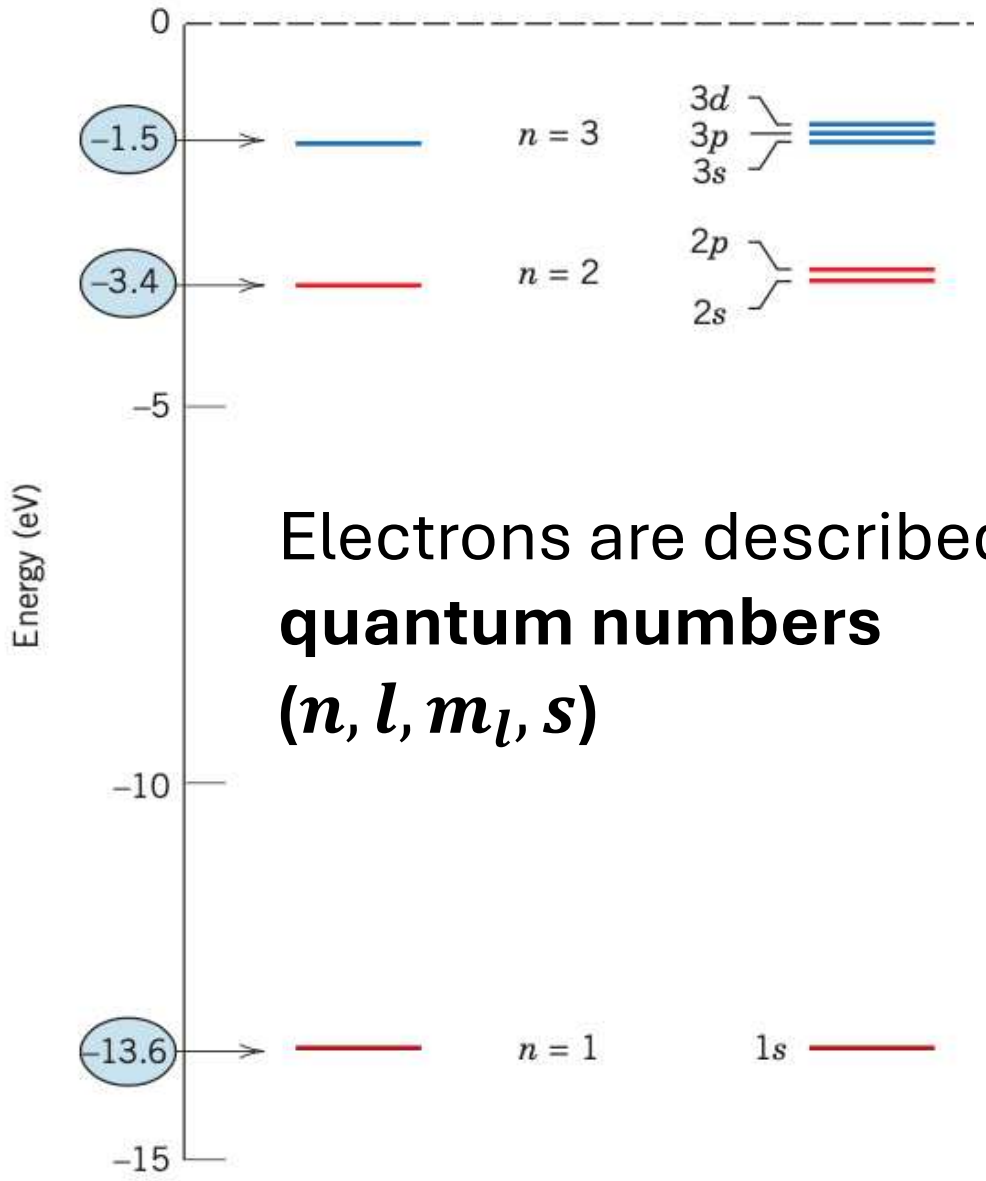
The quantum numbers describing electron orbitals

Principal quantum number (n):

- Specifies the electron **shell**
- $n = 1, 2, 3, \ldots$

→ Further from nucleus

→ Higher in energy



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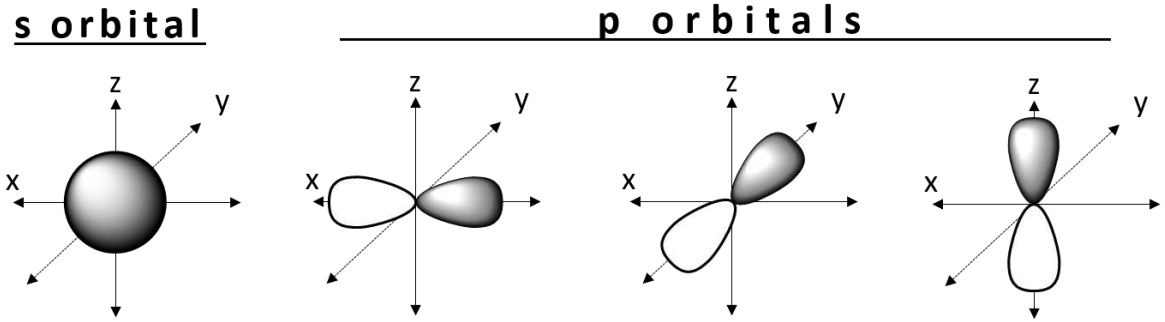
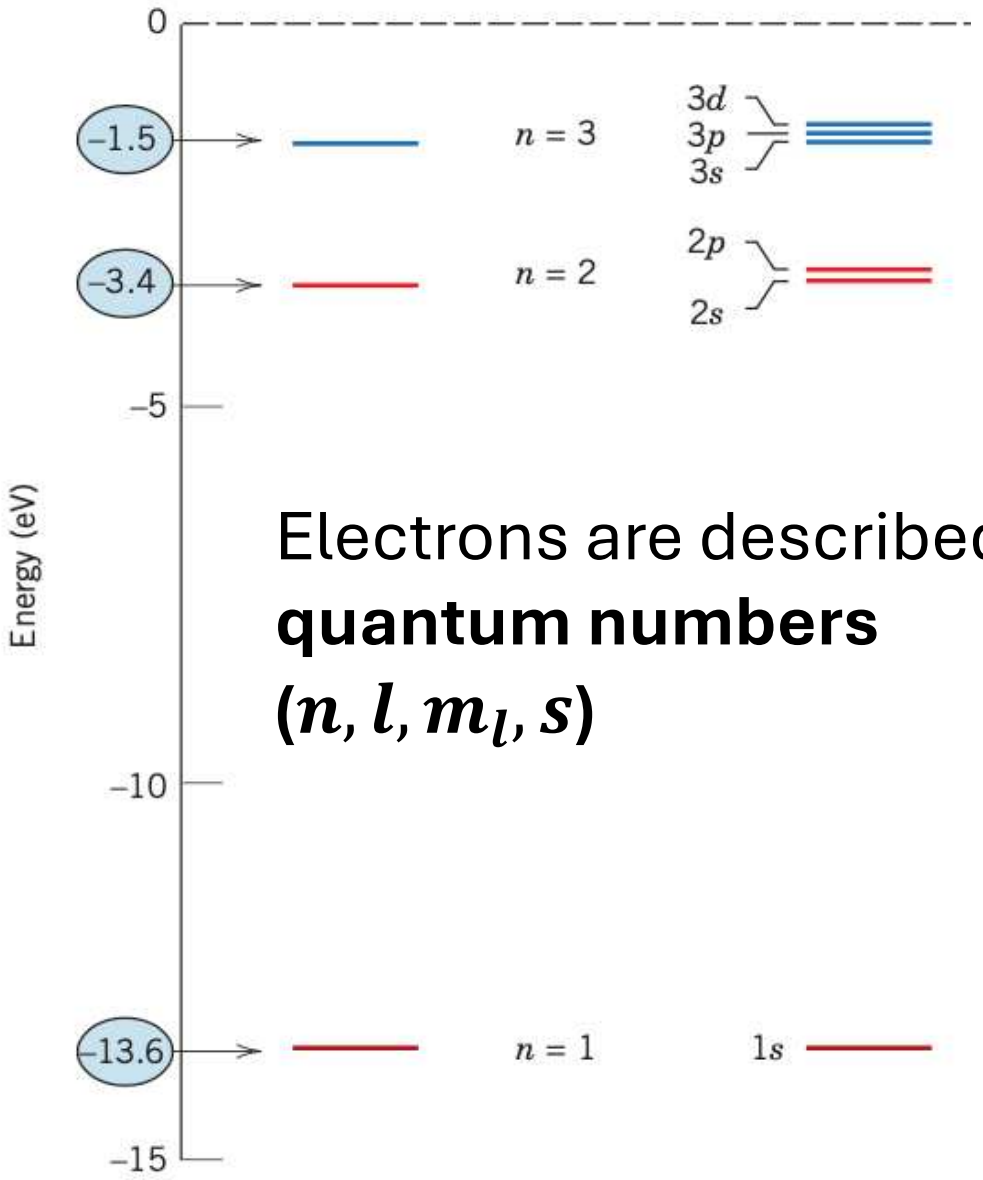
Angular momentum (l):

- Specifies the **subshell**
- $l = 0, 1, \ldots, n-1$

s, p, d, f

These dictate orbital "shape"





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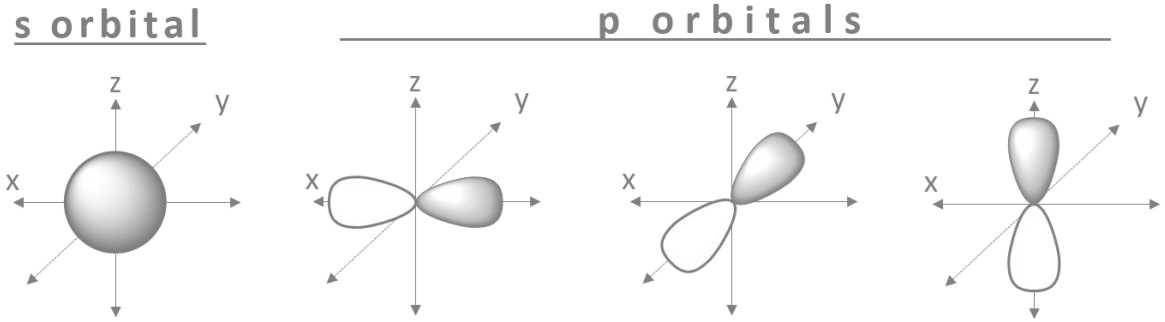
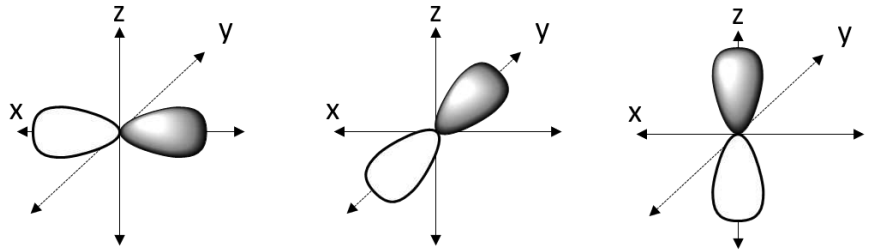


Magnetic quantum number (m_l):

- Specifies the **orbital** in each subshell
- $m_l = -l, \ldots, 0, \ldots, +l$

$l = 1$



$m_l = -1$ $m_l = 0$ $m_l = +1$

The quantum numbers describing electron orbitals

Principal quantum number (n):

- Specifies the electron **shell**
- $n = 1, 2, 3, \ldots$

→ Further from nucleus

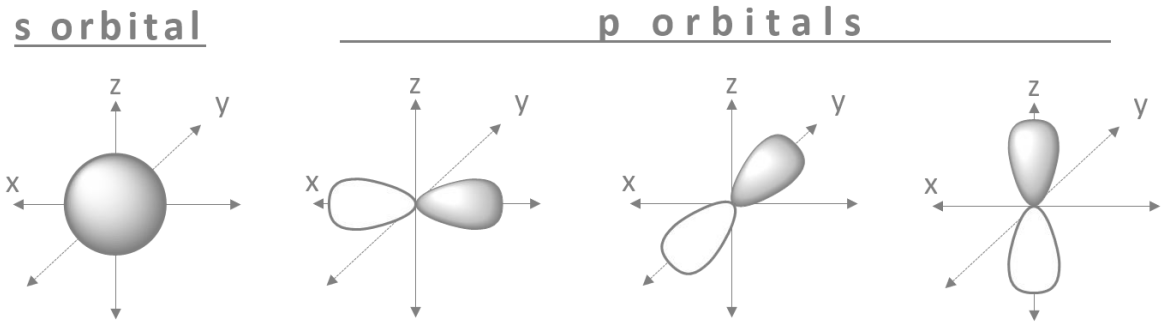
→ Higher in energy

Angular momentum (l):

- Specifies the **subshell**
- $l = 0, 1, \ldots, n-1$

s, p, d, f

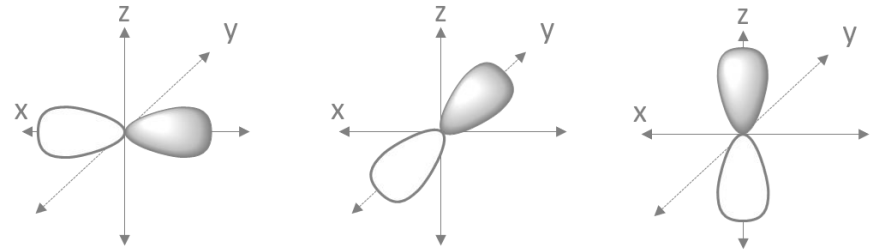
These dictate orbital "shape"



Magnetic quantum number (m_l):

- Specifies the **orbital** in each subshell
- $m_l = -l, \ldots, 0, \ldots, +l,$

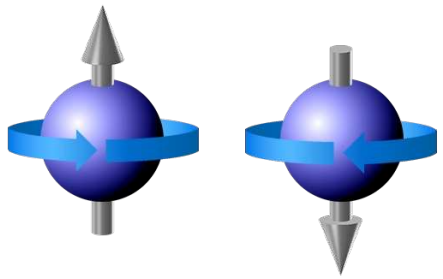
$l = 1$



$m_l = -1$ $m_l = 0$ $m_l = +1$

Spin number (s):

- Specifies the **electron spin**
- $s = +\frac{1}{2}$ (up) or $-\frac{1}{2}$ (down)

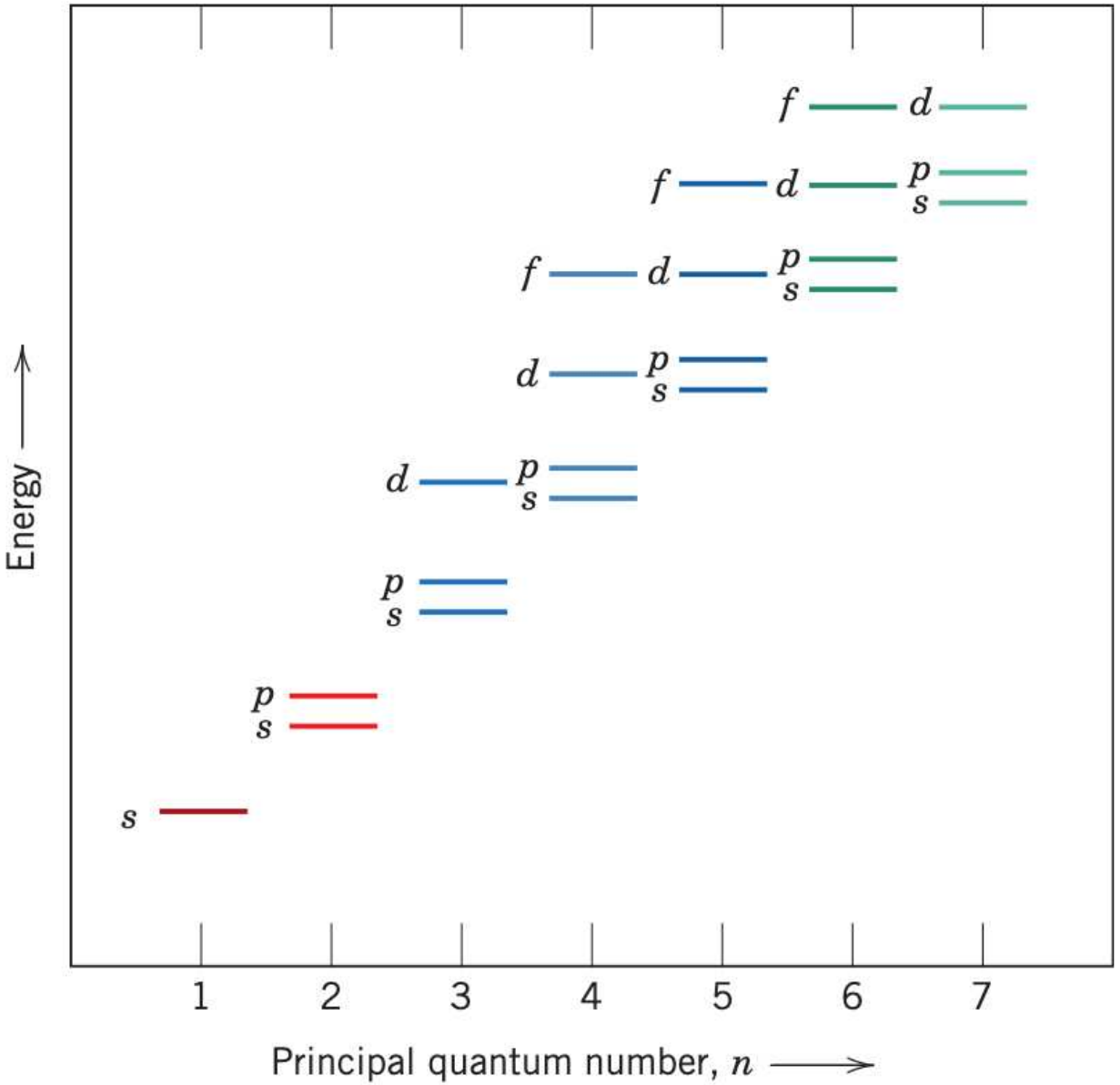


The quantum numbers describing electron orbitals

Table 2.1 Summary of the Relationships among the Quantum Numbers n, l, m_l and Numbers of Orbitals and Electrons

Value of n	*Value of l*	*Values of m_l*	*Subshell*	*Number of Orbitals*	*Number of Electrons*
1	0	0	1*s*	1	2
2	0	0	2*s*	1	2
	1	−1, 0, +1	2*p*	3	6
3	0	0	3*s*	1	2
	1	−1, 0, +1	3*p*	3	6
	2	−2, −1, 0, +1, +2	3*d*	5	10
4	0	0	4*s*	1	2
	1	−1, 0, +1	4*p*	3	6
	2	−2, −1, 0, +1, +2	4*d*	5	10
	3	−3, −2, −1, 0, +1, +2, +3	4*f*	7	14

These orbitals are filled in order of increasing energy



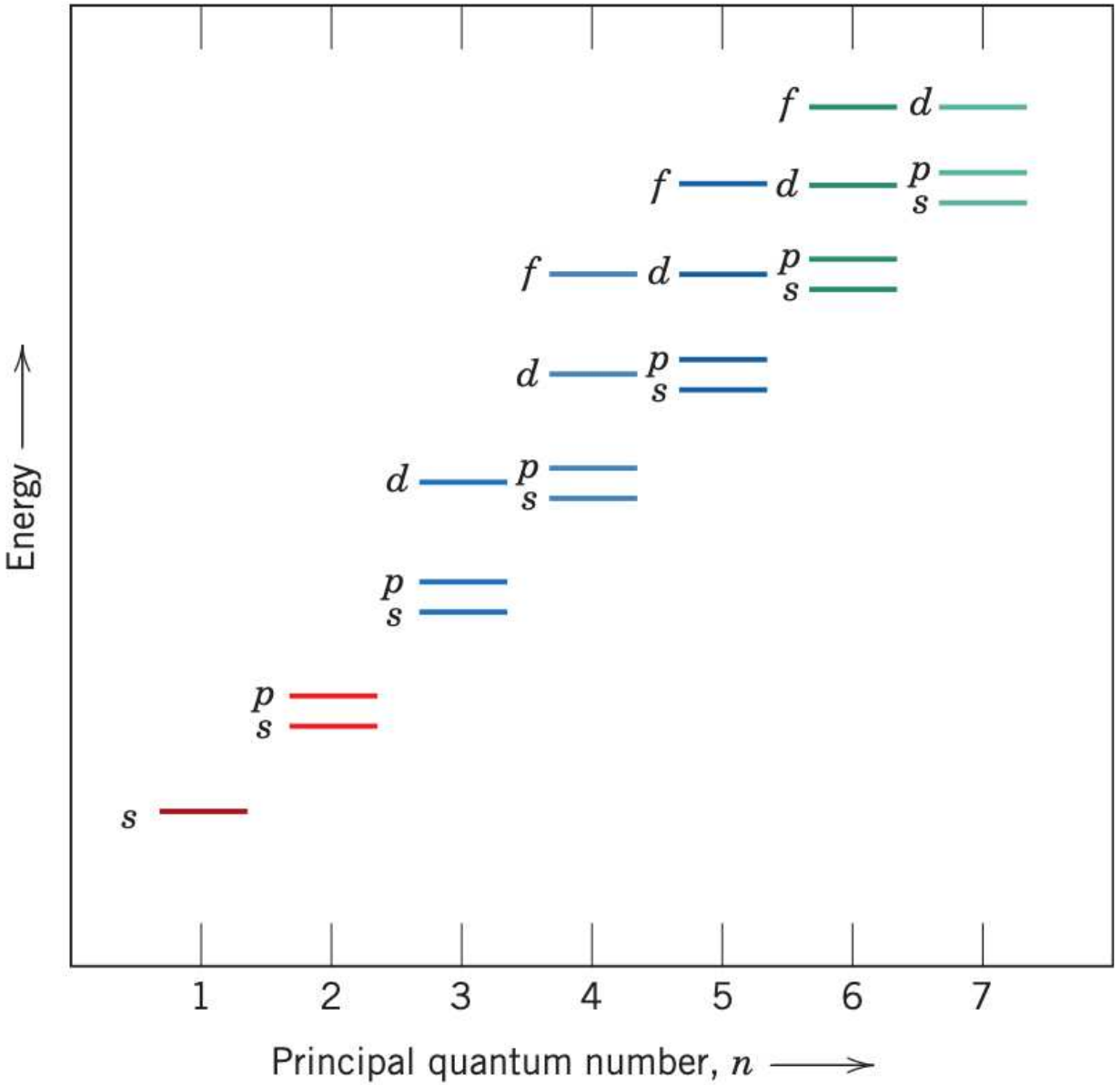
- The principal quantum number (n) largely dictates energy, with smaller differences between subshells (l)

- Electrons in an atom want to fill the lowest-energy orbitals first while **obeying Pauli exclusion principle**

No two electrons in an atom can have the same set of quantum numbers.

→ 2 electrons (spin up/down) can occupy each orbital

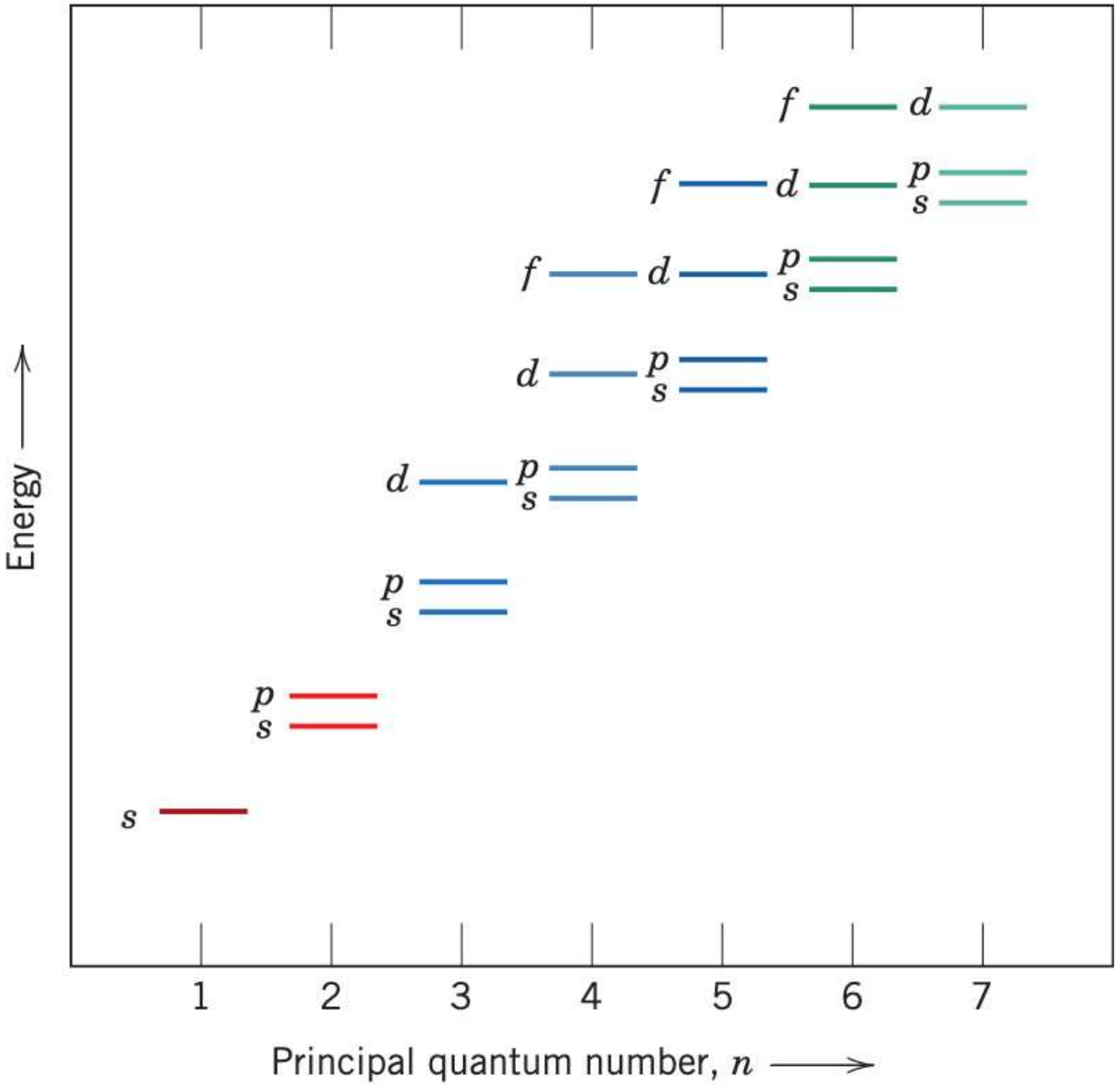
These orbitals are filled in order of increasing energy





What is the electron configuration of sodium?

These orbitals are filled in order of increasing energy

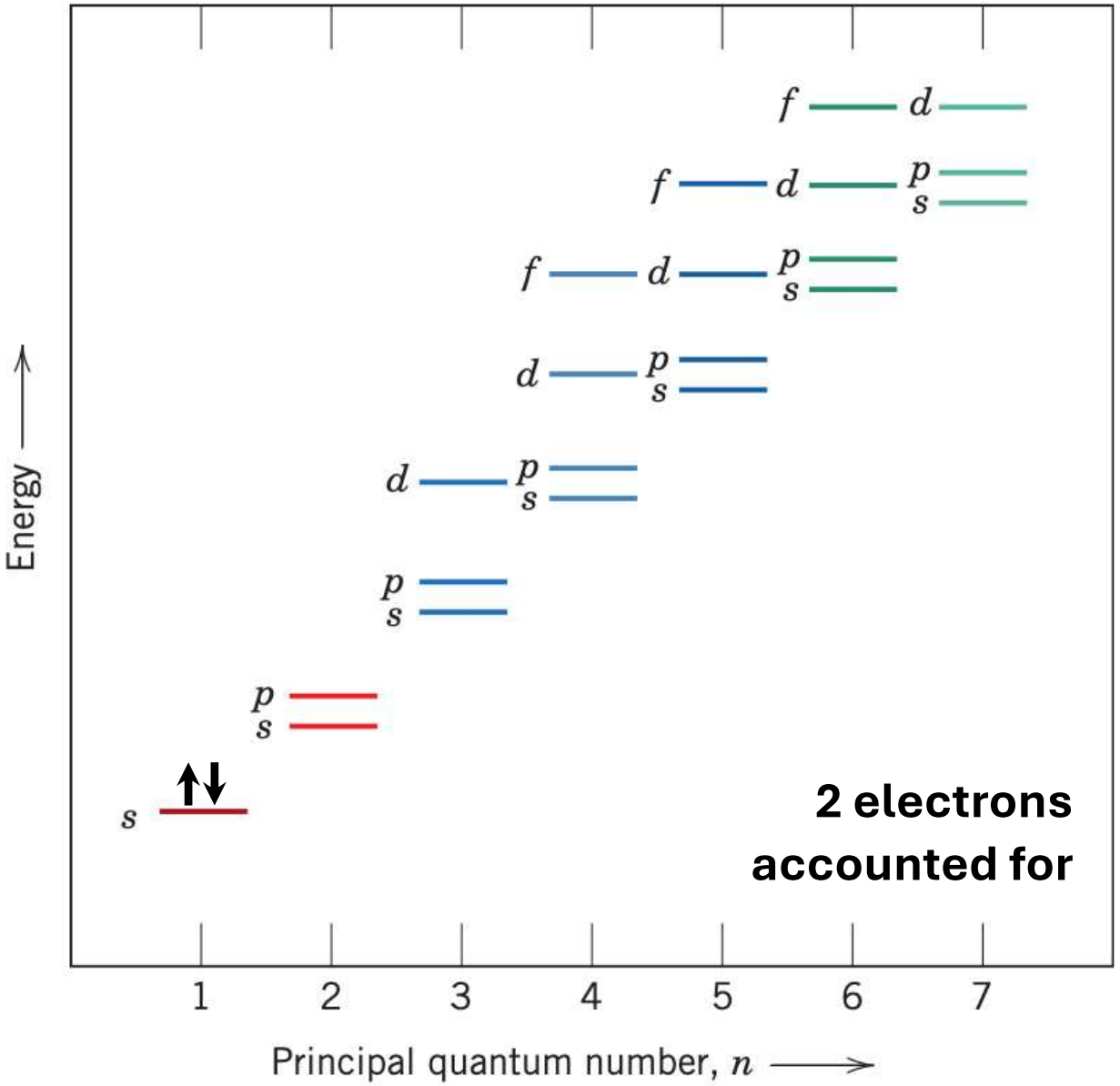




What is the electron configuration of sodium?

11 total electrons:

These orbitals are filled in order of increasing energy



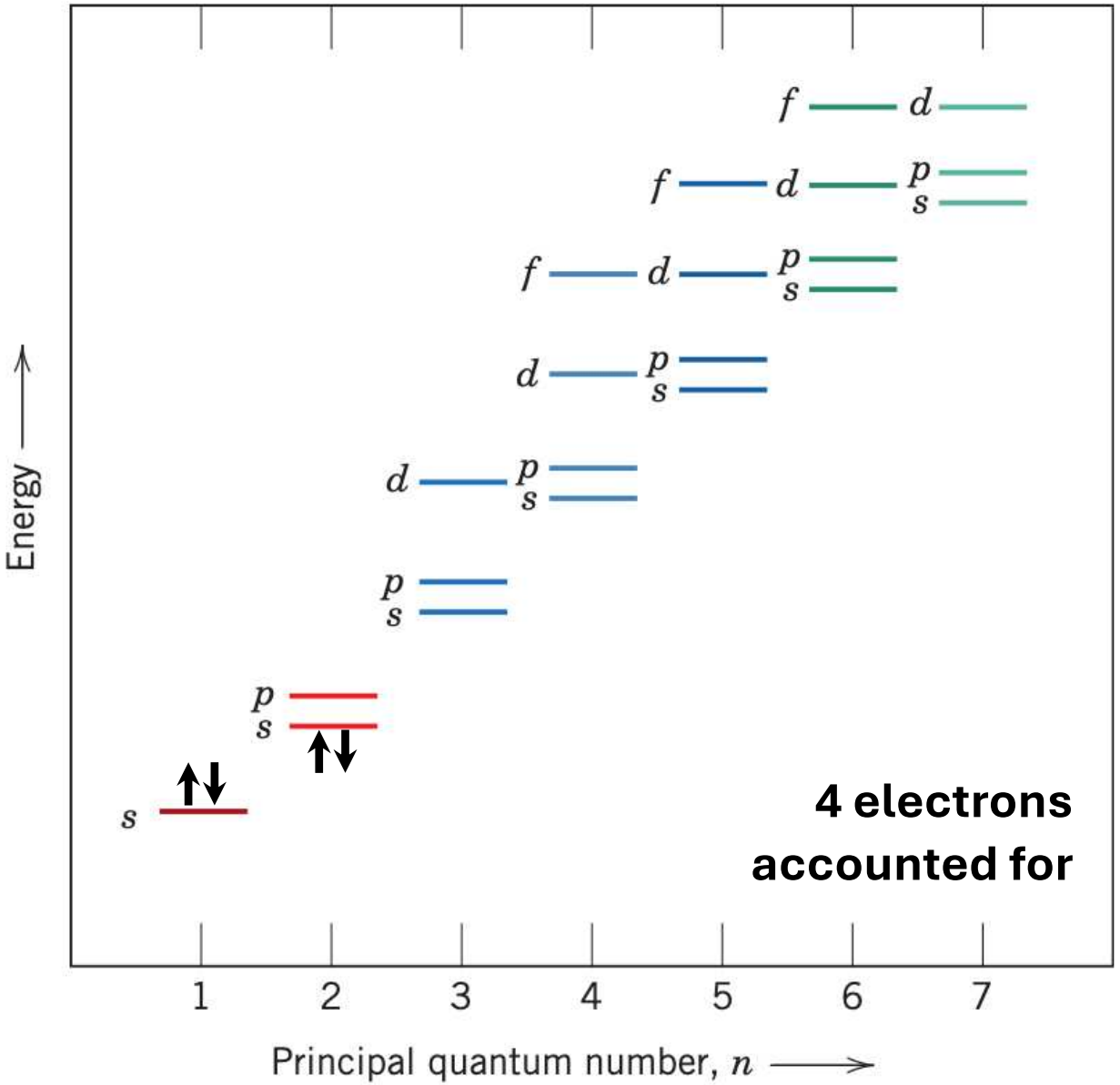


What is the electron configuration of sodium?

11 total electrons:

- 2 electrons in 1s orbital

These orbitals are filled in order of increasing energy



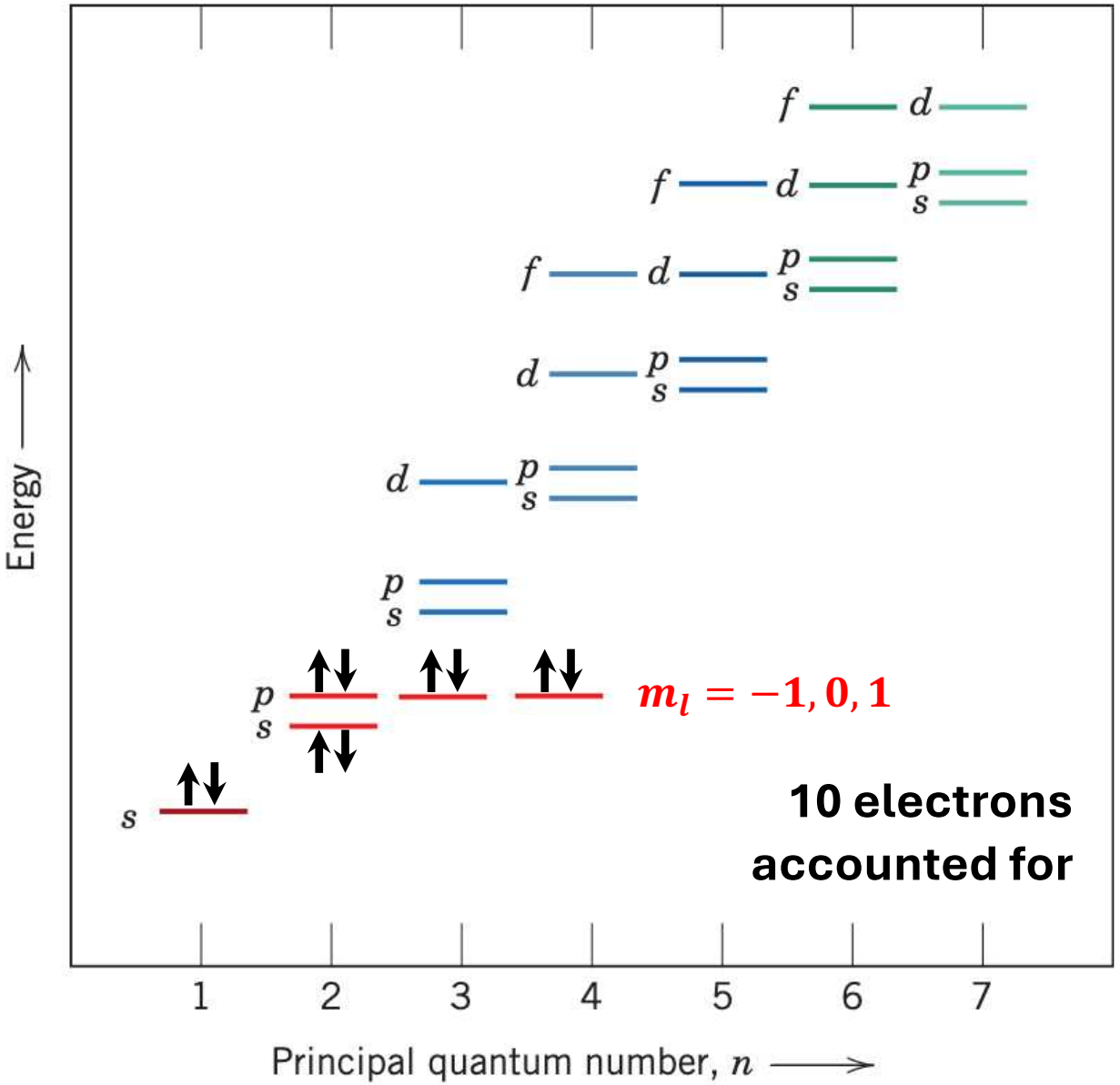


What is the electron configuration of sodium?

11 total electrons:

- 2 electrons in 1s orbital
- 2 electrons in 2s orbital

These orbitals are filled in order of increasing energy



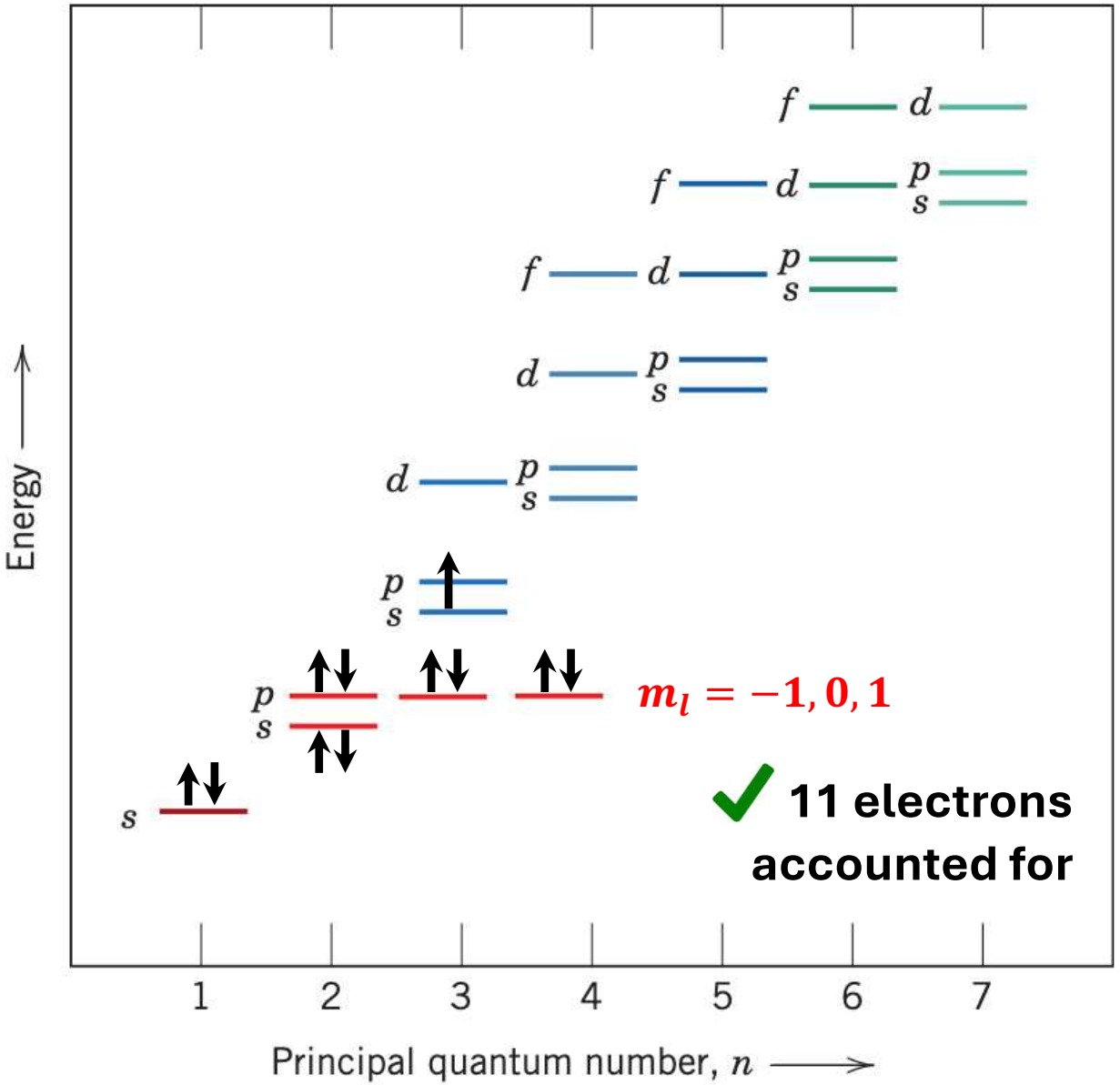


What is the electron configuration of sodium?

11 total electrons:

- 2 electrons in 1s orbital
- 2 electrons in 2s orbital
- 6 electrons in 2p orbitals

These orbitals are filled in order of increasing energy



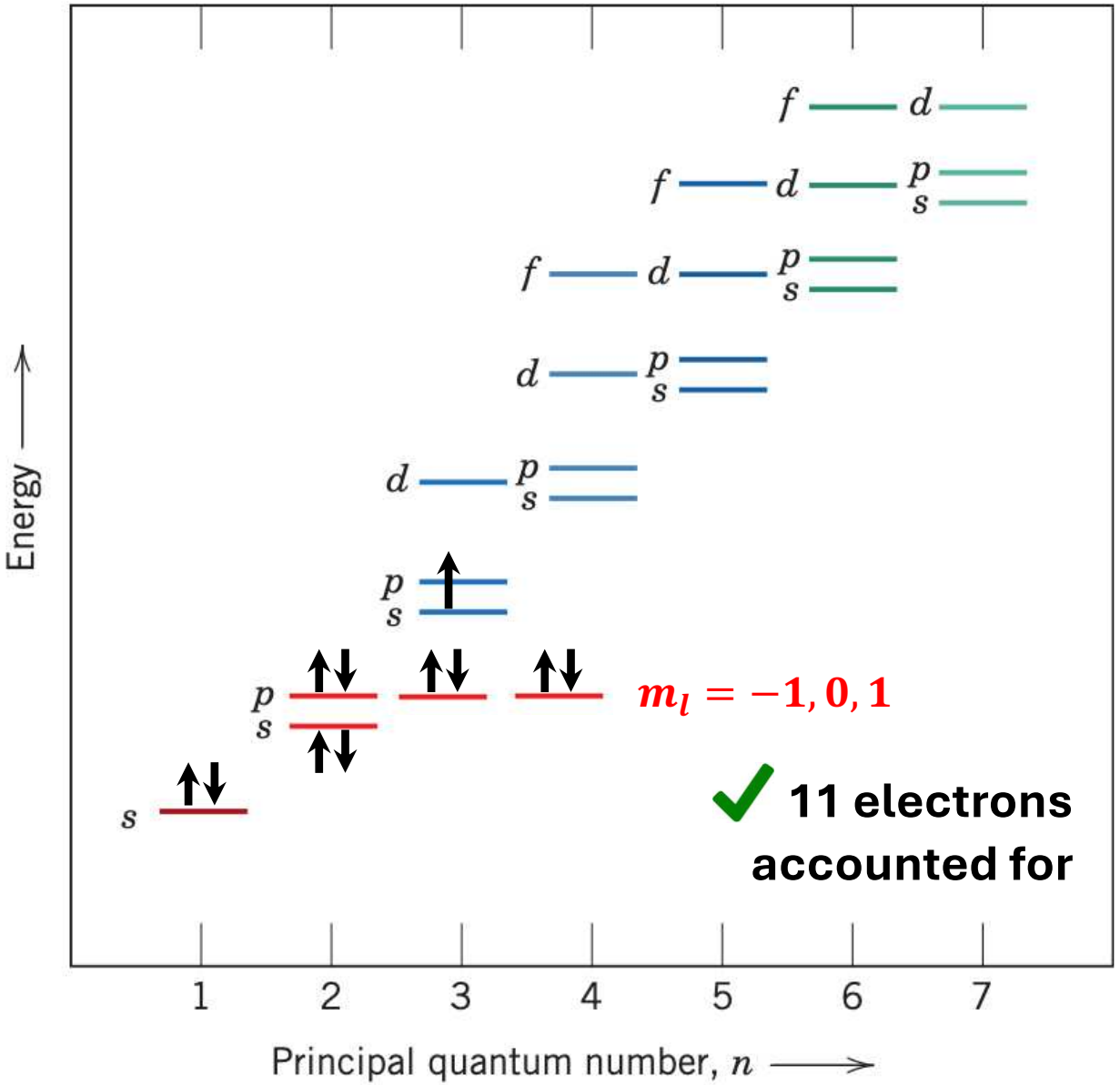


What is the electron configuration of sodium?

11 total electrons:

- 2 electrons in 1s orbital
- 2 electrons in 2s orbital
- 6 electrons in 2p orbital
- 1 electron in 3s orbital

These orbitals are filled in order of increasing energy





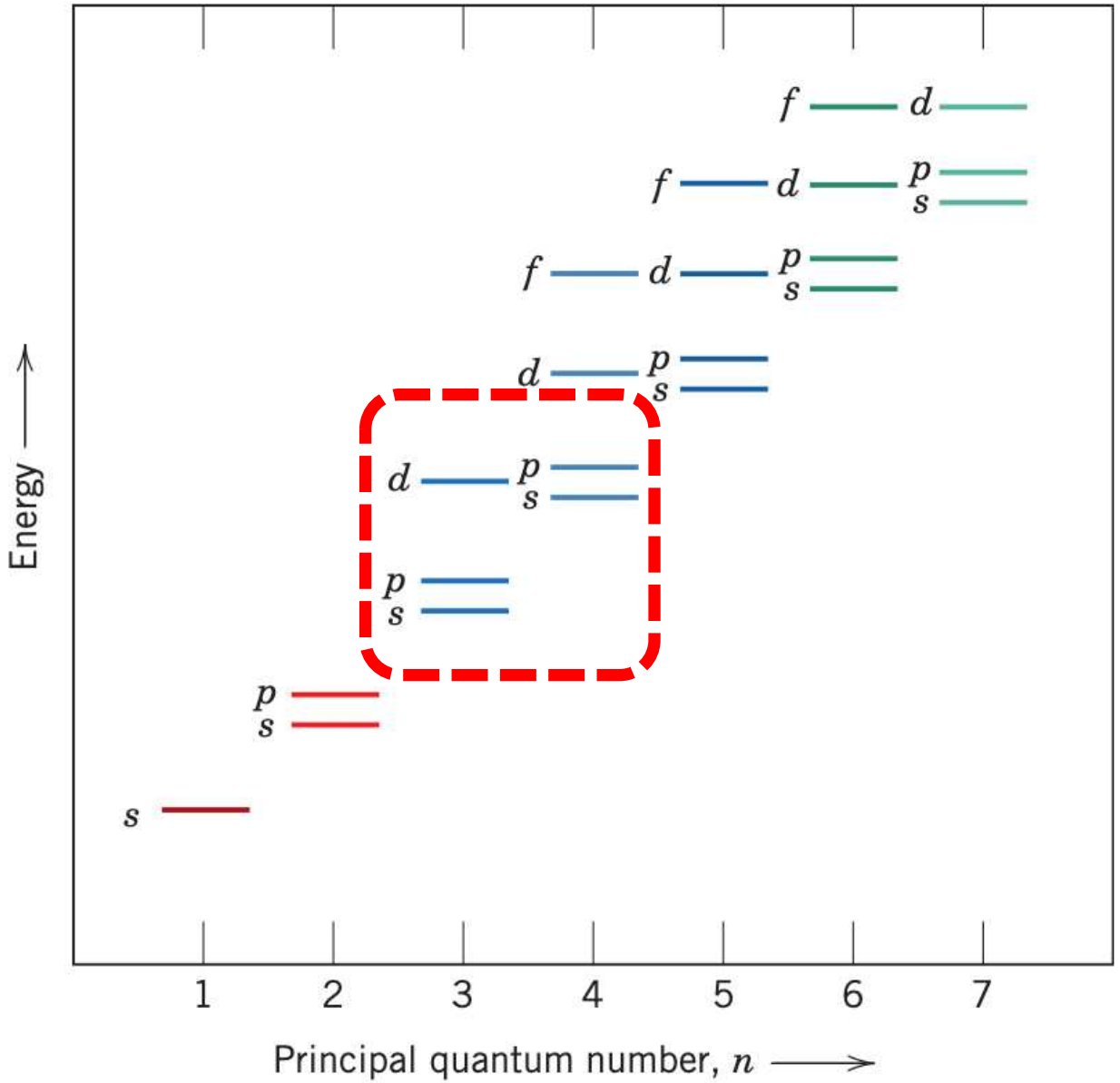
What is the electron configuration of sodium?

11 total electrons:

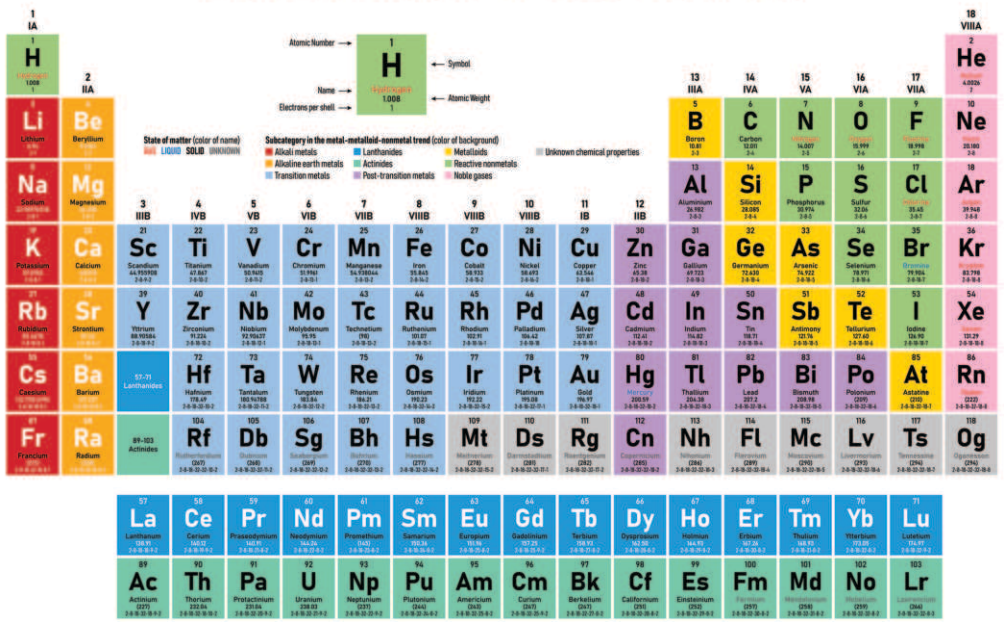
- 2 electrons in 1s orbital
- 2 electrons in 2s orbital
- 6 electrons in 2p orbital
- 1 electron in 3s orbital

Configuration: $1s^2 2s^2 2p^6 3s^1$

These orbitals are filled in order of increasing energy

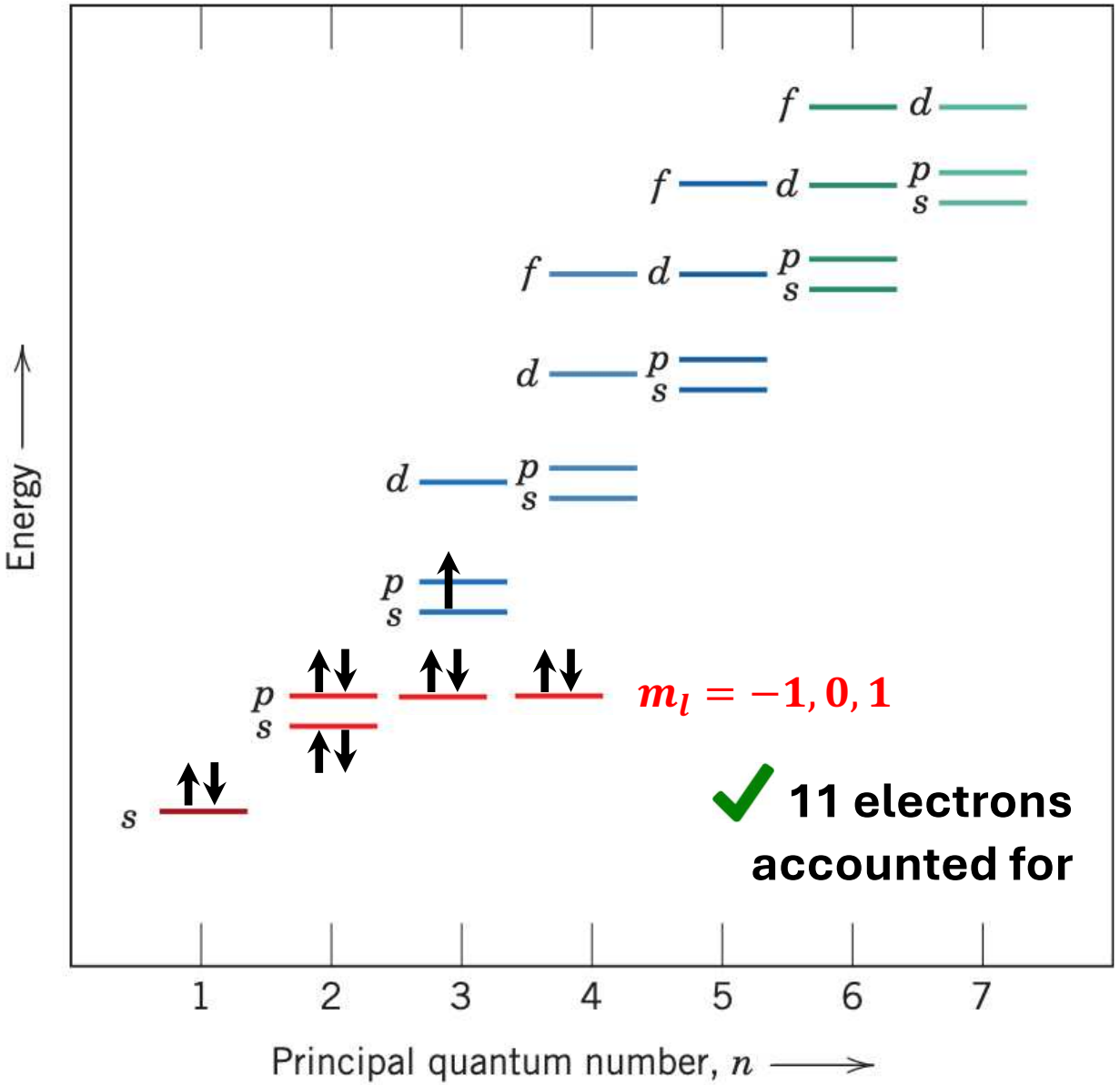


One subtlety: we fill the 4s orbitals before the 3d orbitals



Ti: $1s^2 2s^2 2p^6 3s^2 3p^6 \mathbf{4s^2 3d^2}$

These orbitals are filled in order of increasing energy





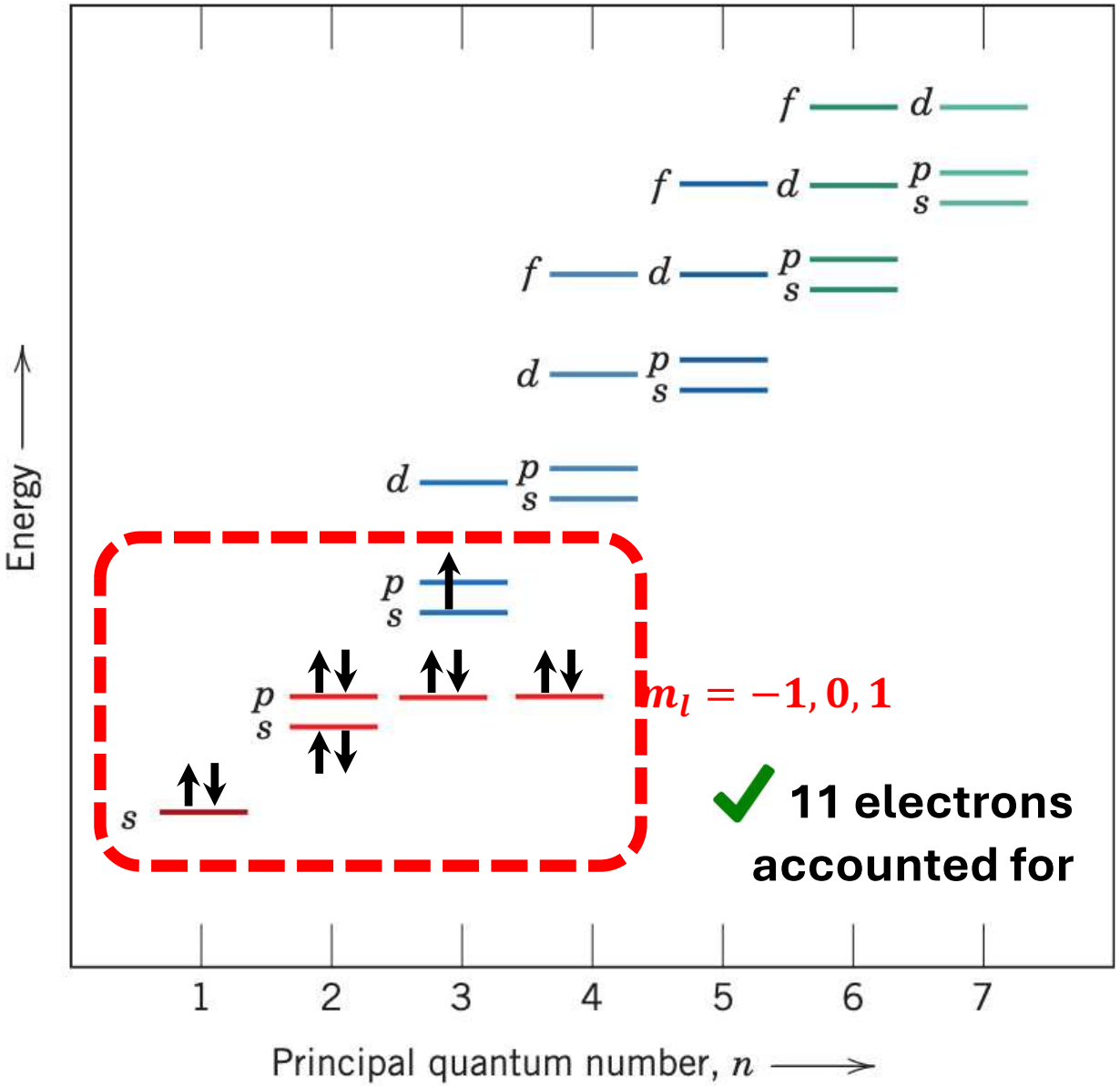
What is the electron configuration of sodium?

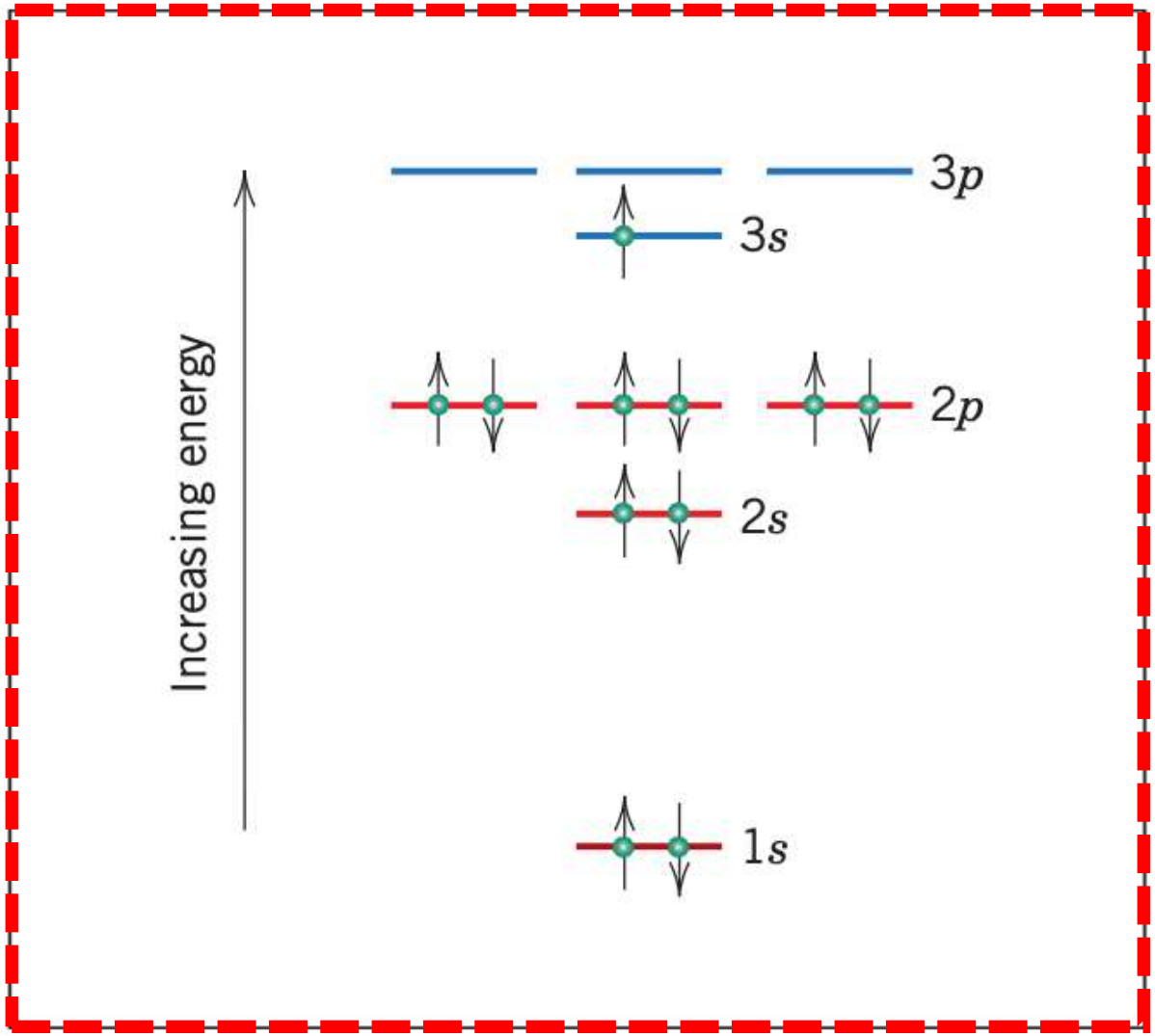
11 total electrons:

- 2 electrons in 1s orbital
- 2 electrons in 2s orbital
- 6 electrons in 2p orbital
- 1 electron in 3s orbital

Configuration: $1s^2 2s^2 2p^6 3s^1$

These orbitals are filled in order of increasing energy





Back to Na: $1s^2 2s^2 2p^6 3s^1$

These orbitals are filled in order of increasing energy

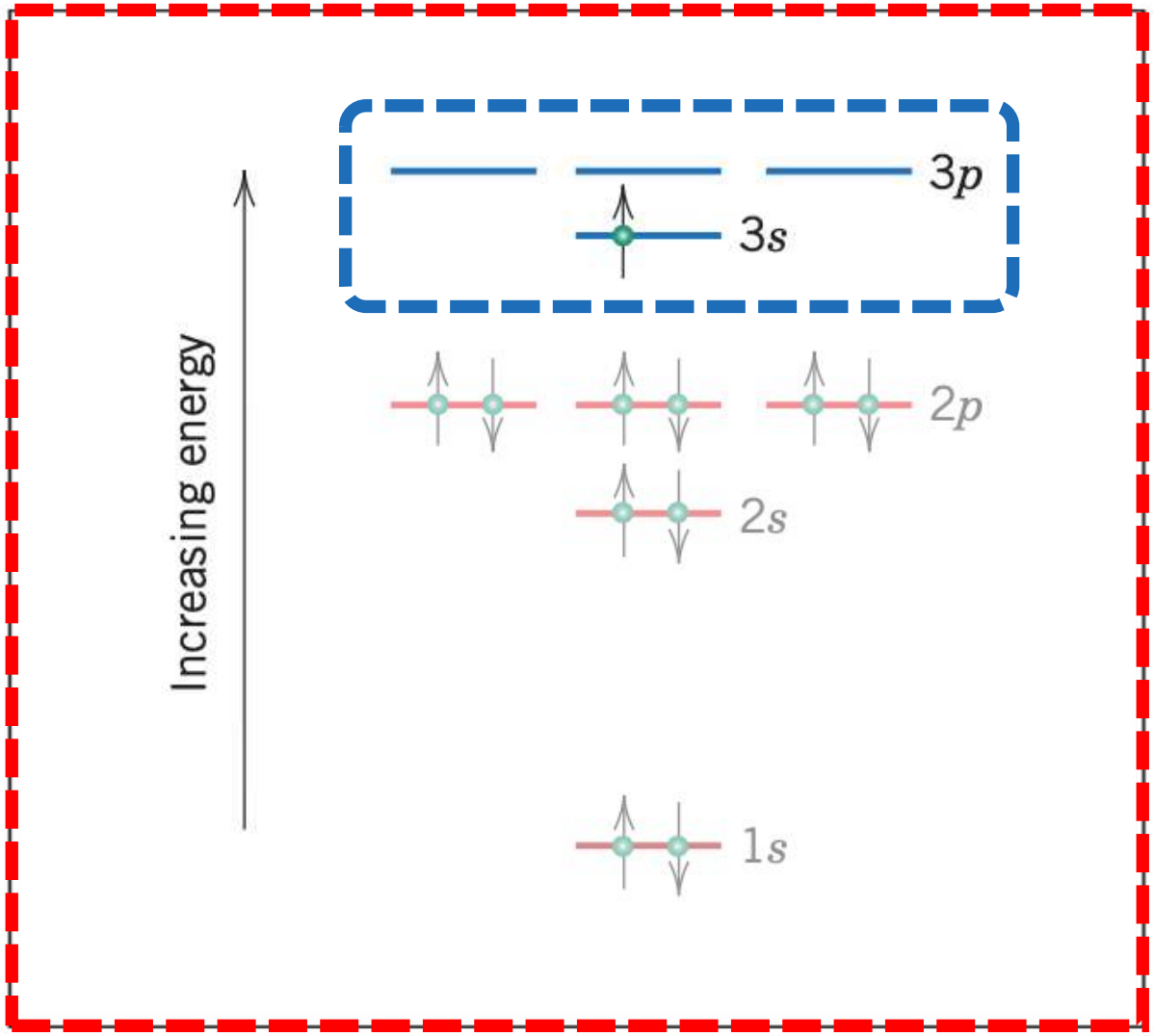
It is the electrons in the outermost shell – the **valence electrons** – that we typically care about
→ **These dictate bonding**

Octet rule: atoms are "happiest" (most stable) when their outermost shell is completely filled

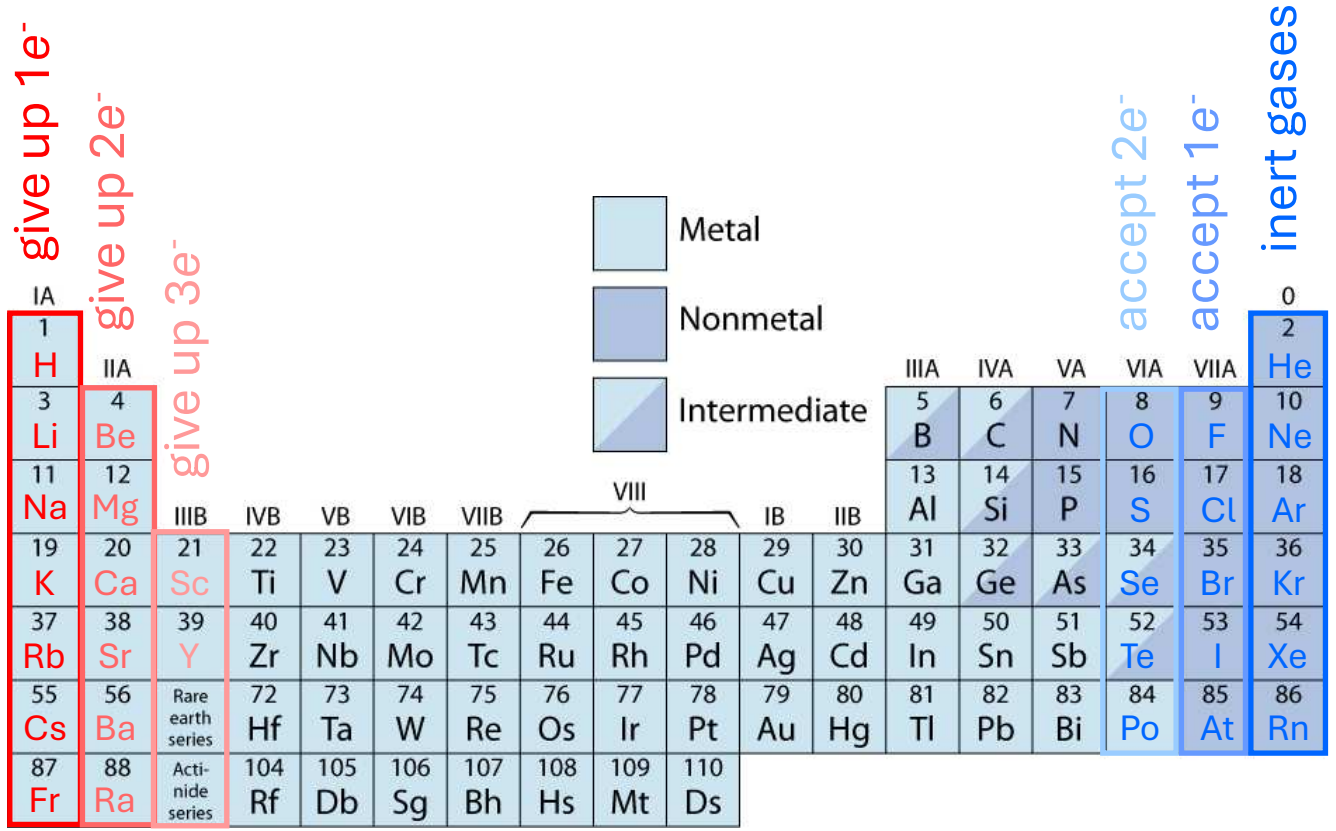
They accomplish this either by:

Gaining **valence electrons**

Losing **valence electrons**



Electronegativity: whether to gain/lose electrons



Cations

Anions

Electropositive elements:
Readily give up electrons
to become + ions.

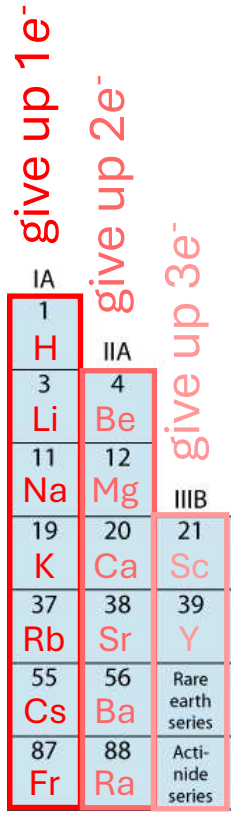
Smaller electronegativity

Electronegative elements:
Readily acquire electrons
to become - ions.

Larger electronegativity

Electronegativity: whether to gain/lose electrons

Cations



Electropositive elements:
Readily give up electrons
to become + ions.

Smaller electronegativity

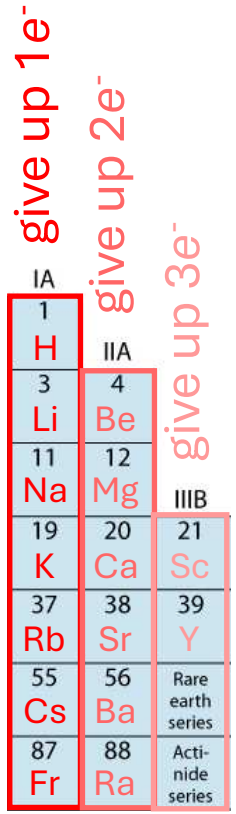
Example:

Na: $1s^2 2s^2 2p^6 3s^1$

Na^+: $1s^2 2s^2 2p^6 3s^0$

Electronegativity: whether to gain/lose electrons

Cations



Electropositive elements:
Readily give up electrons
to become + ions.

Smaller electronegativity

Example:

Na: $1s^2 2s^2 2p^6 3s^1$

Na^+: $1s^2 2s^2 2p^6 3s^0$

One more subtlety: transition metals tend to lose their s electrons first*

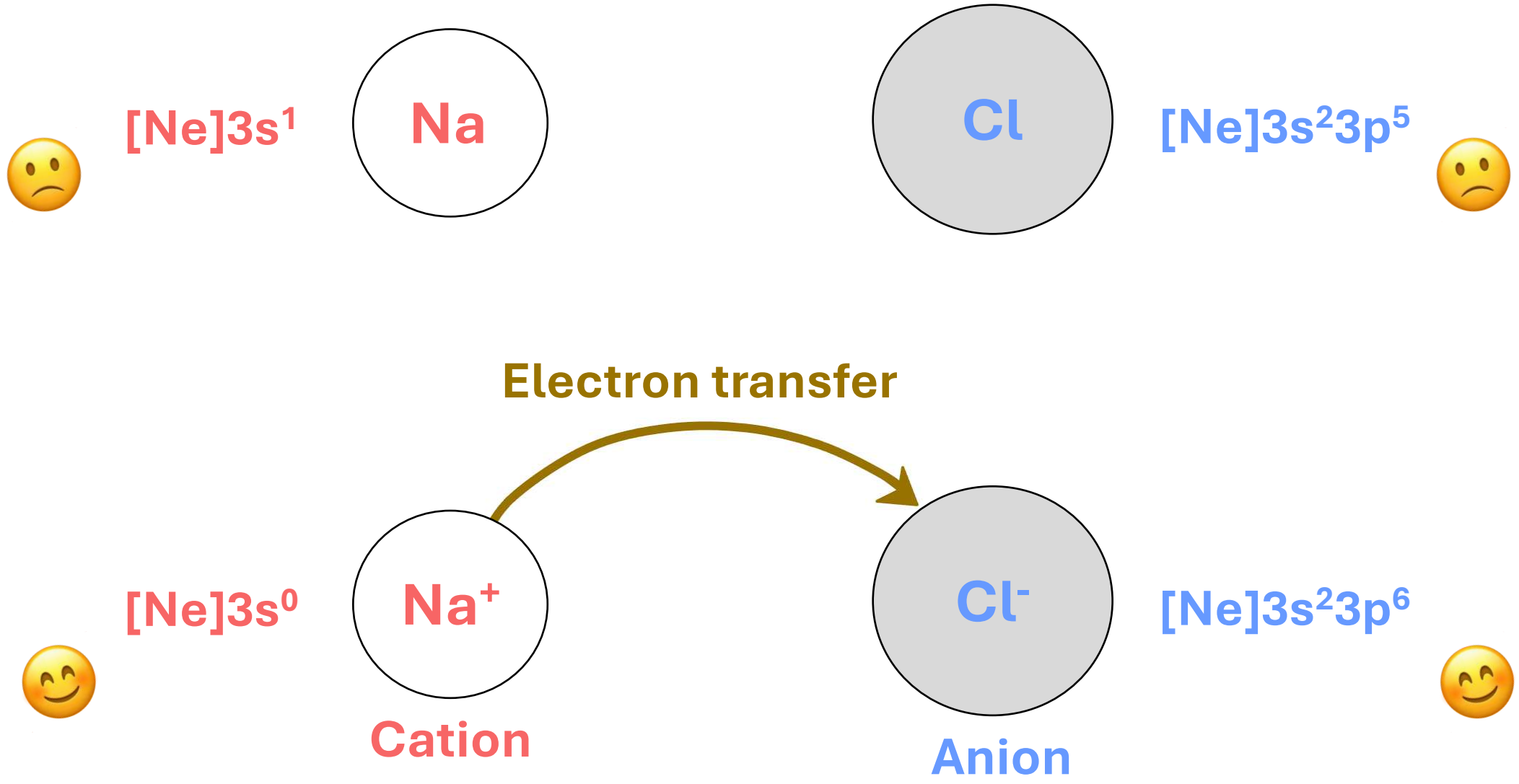
Ti: $1s^2 2s^2 2p^6 3s^2 3p^6 \mathbf{4s^2 3d^2}$

Ti^{2+}: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^0 \mathbf{3d^2}$

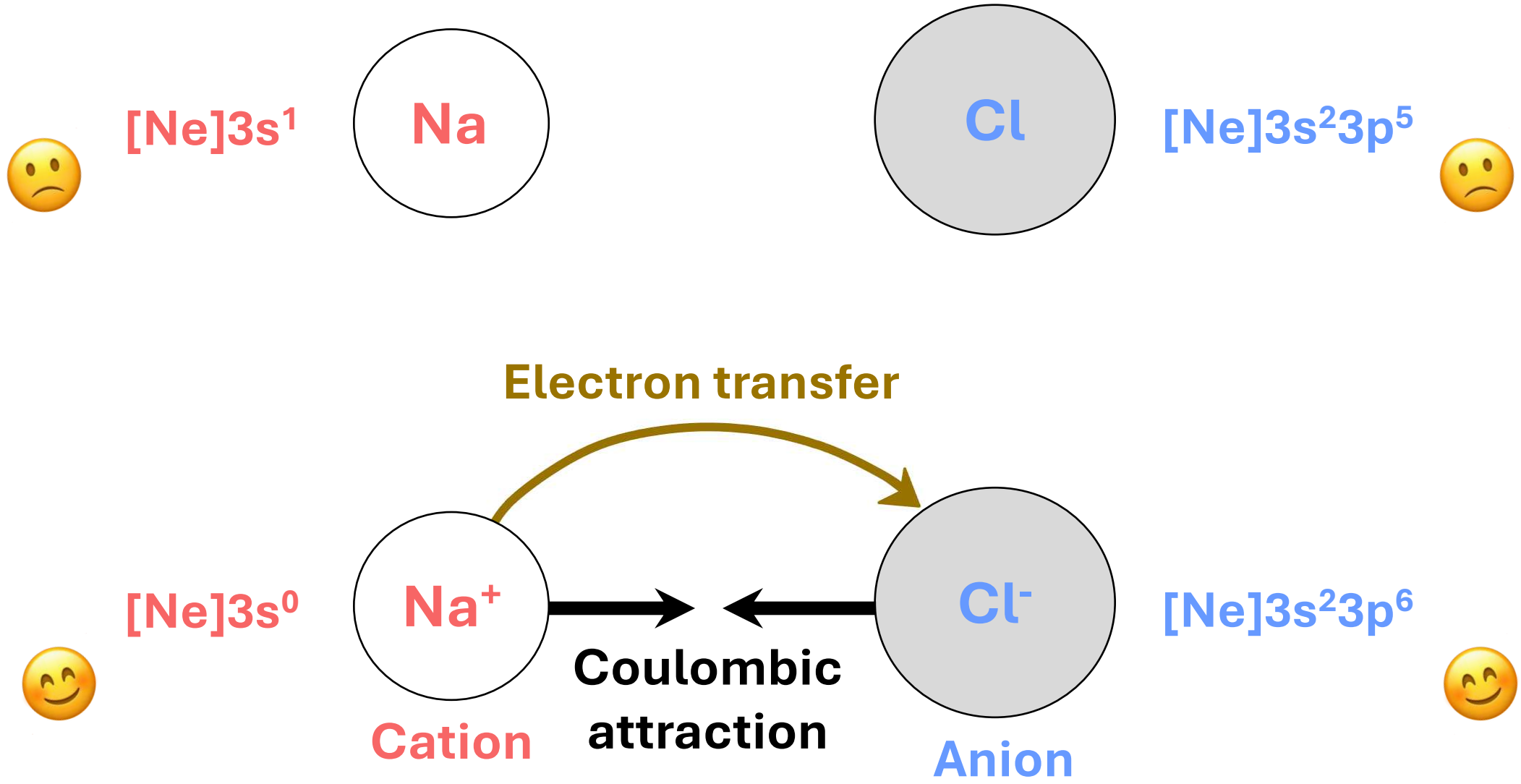
Ti^{4+}: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^0 3d^0$

*Due to screening effects of tightly bound d electrons

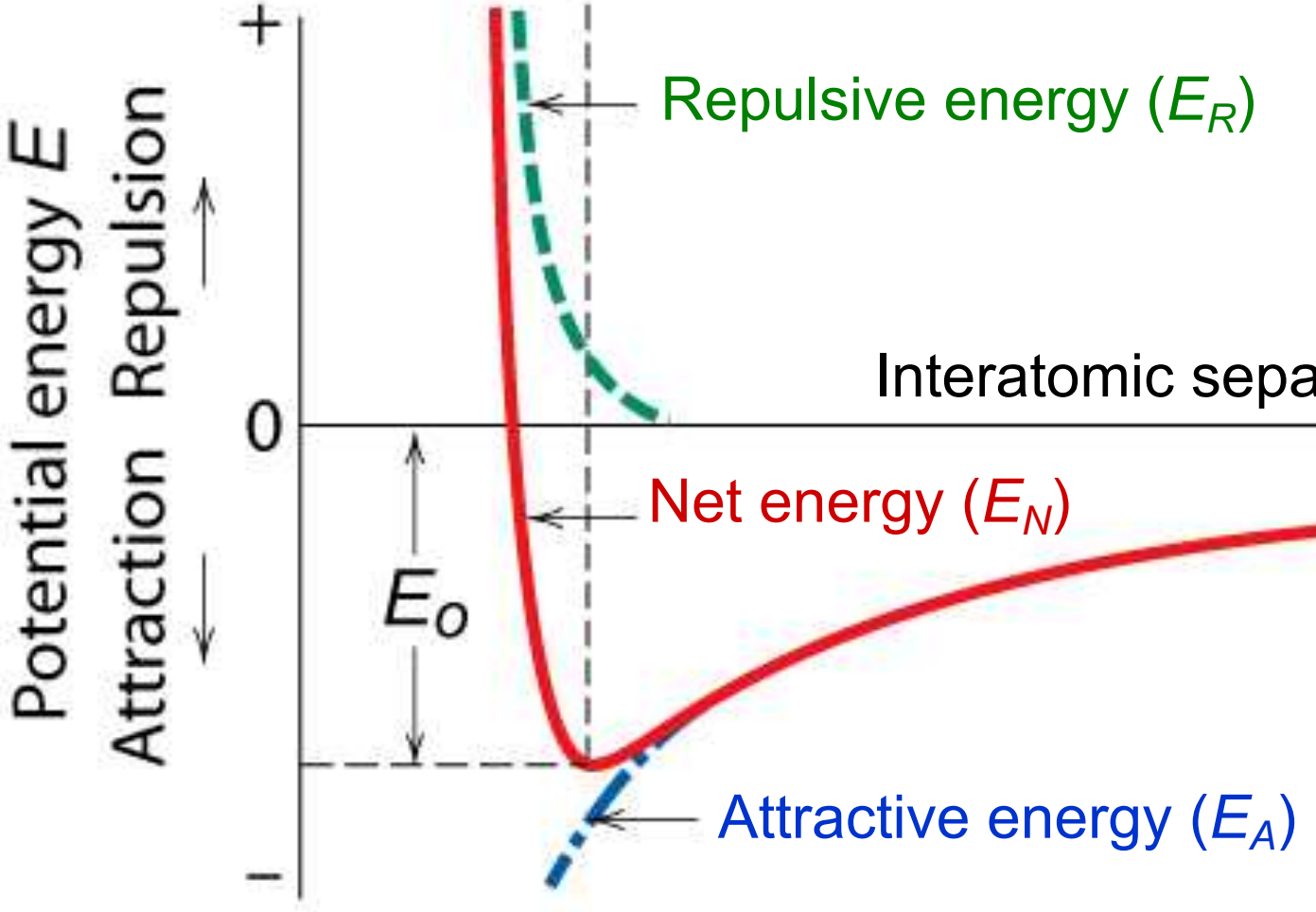
Ionic bonding: cation + anion



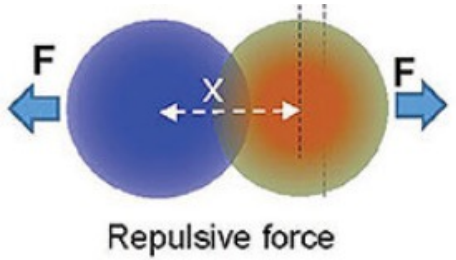
Ionic bonding: cation + anion



Energy balance in ionic bonds



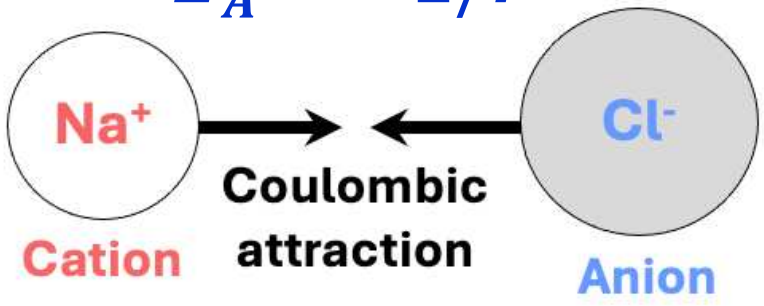
$$E_R \propto +1/r^n \ (n \sim 8)$$



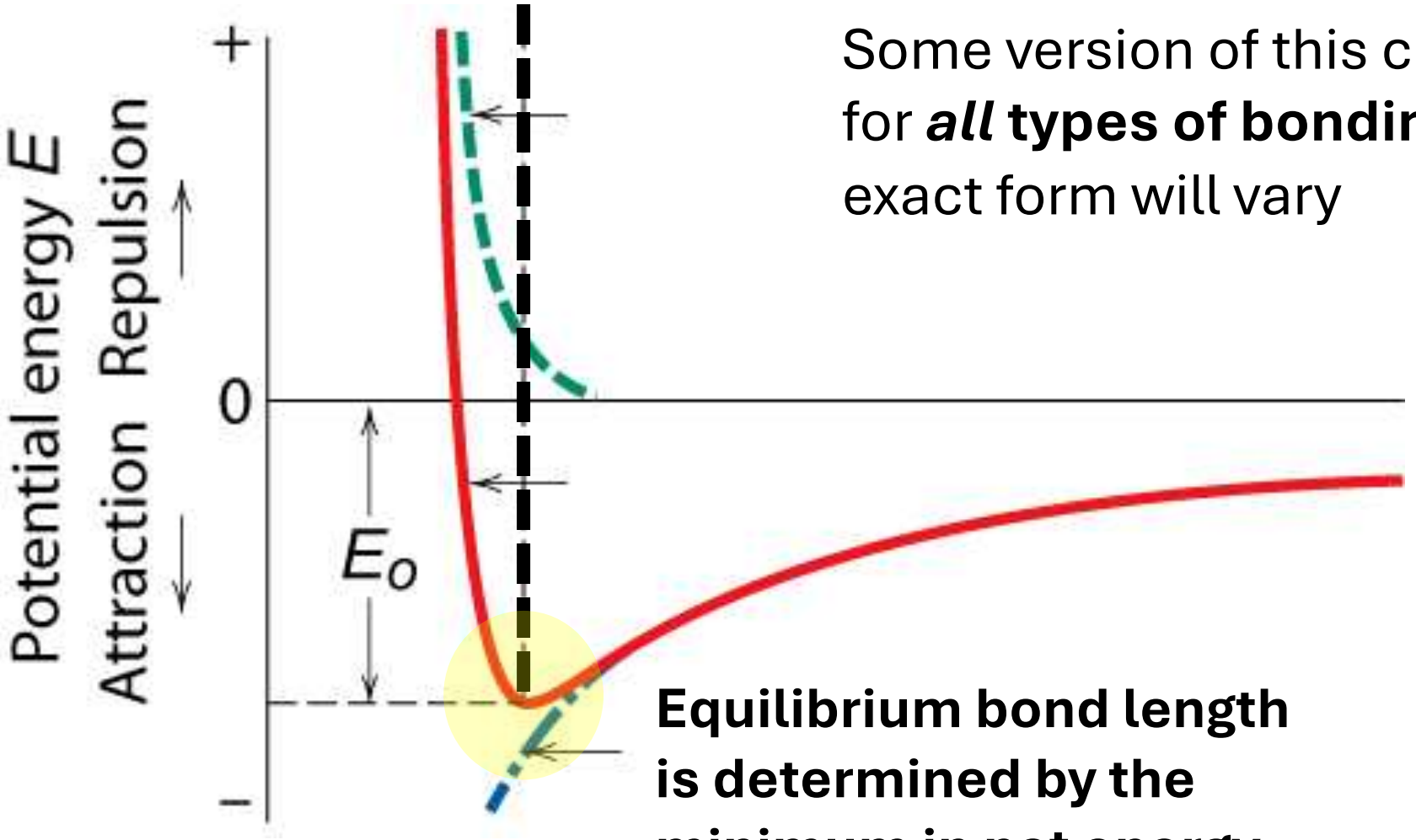
Recall: Pauli exclusion!

$$E_N = \frac{A}{r^n} - \frac{B}{r}$$

$$E_A \propto -1/r$$



Energy balance in ionic bonds

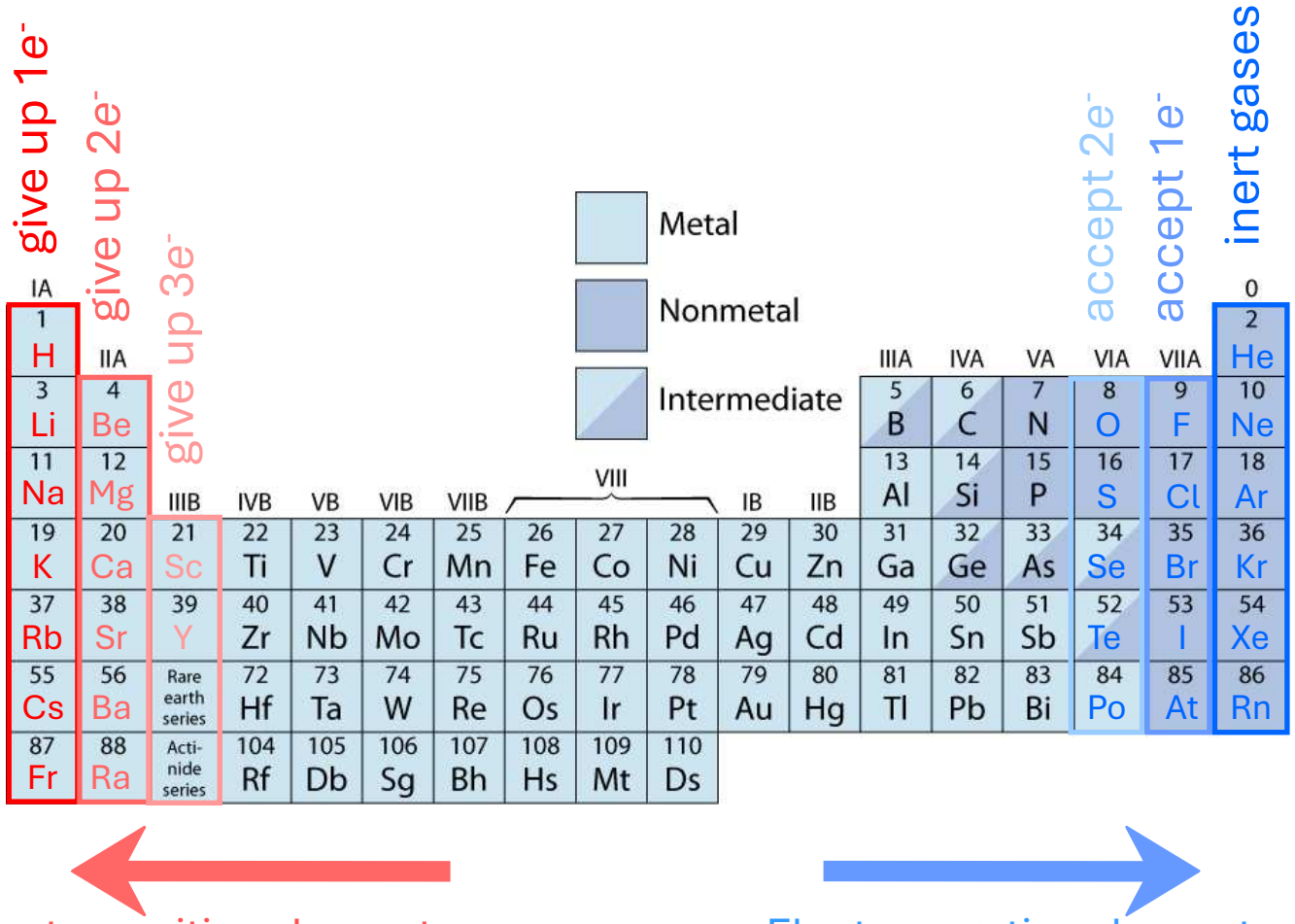


Some version of this curve exists for ***all* types of bonding** – the exact form will vary

$$E_N = \frac{A}{r^n} - \frac{B}{r}$$

Equilibrium bond length is determined by the minimum in net energy

Ionic versus covalent bonding



Electropositive elements:
Readily give up electrons
to become + ions.

Smaller electronegativity

Electronegative elements:
Readily acquire electrons
to become - ions.

Larger electronegativity

Ionic bonds form between elements on the **left side (electropositive)** and **right side (electronegative)** of the periodic table

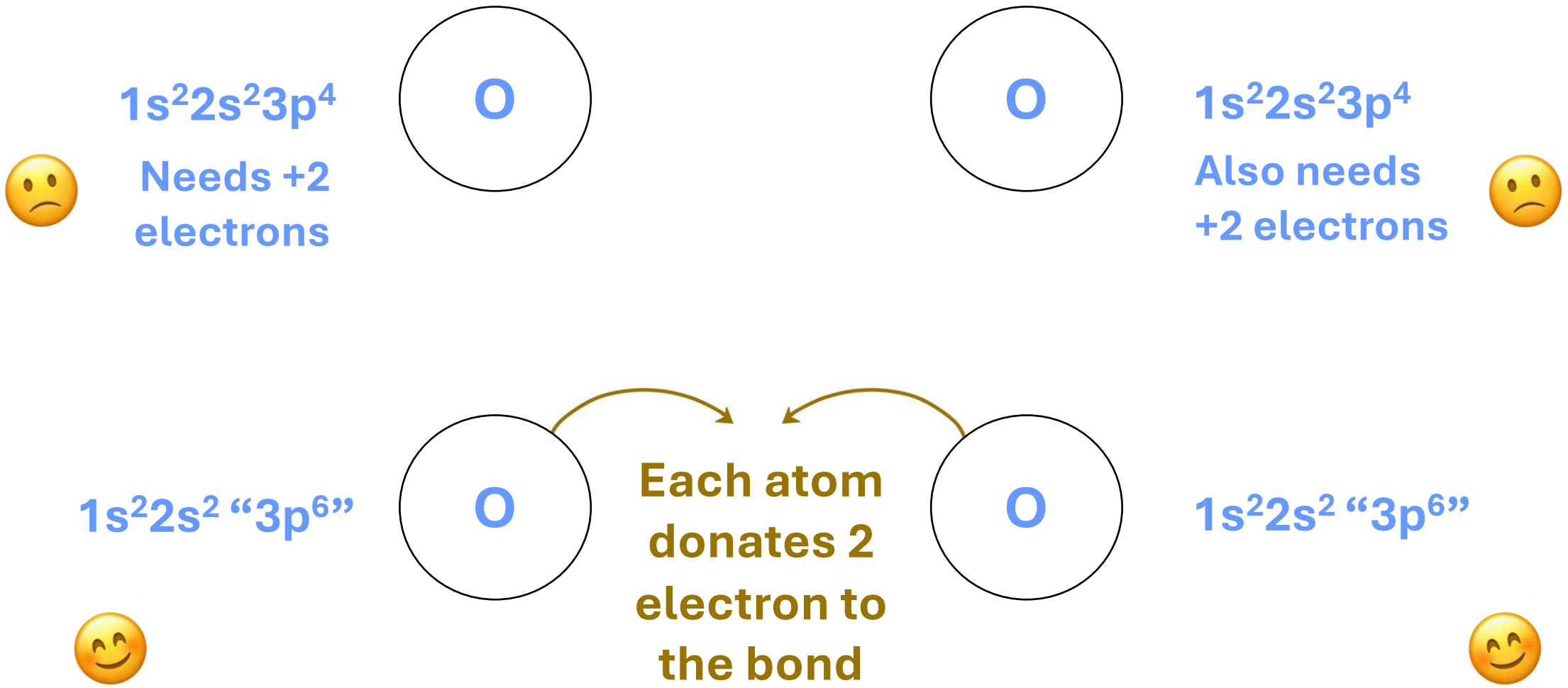
- **Examples:** NaCl, MgO, BaS, CaF_2

What if we combine elements that have **similar electronegativity?**

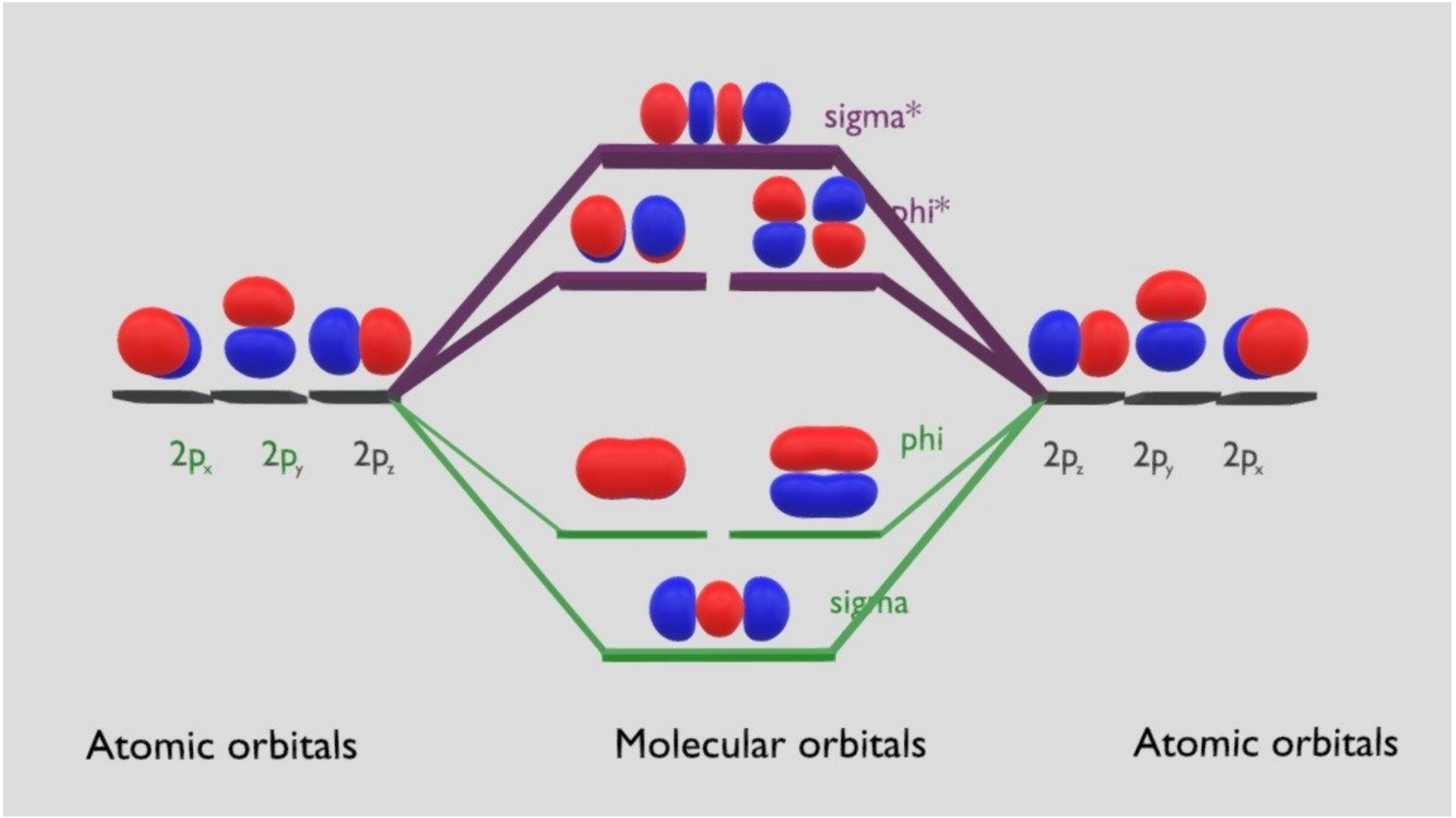
They will ***share* valence electrons** as opposed to completely transferring them → **covalent bond**

- **Examples:** SiC, O_2, GaAs, P_2O_5

Covalent bonding results from electron *sharing*



Covalent bonds result in molecular orbitals

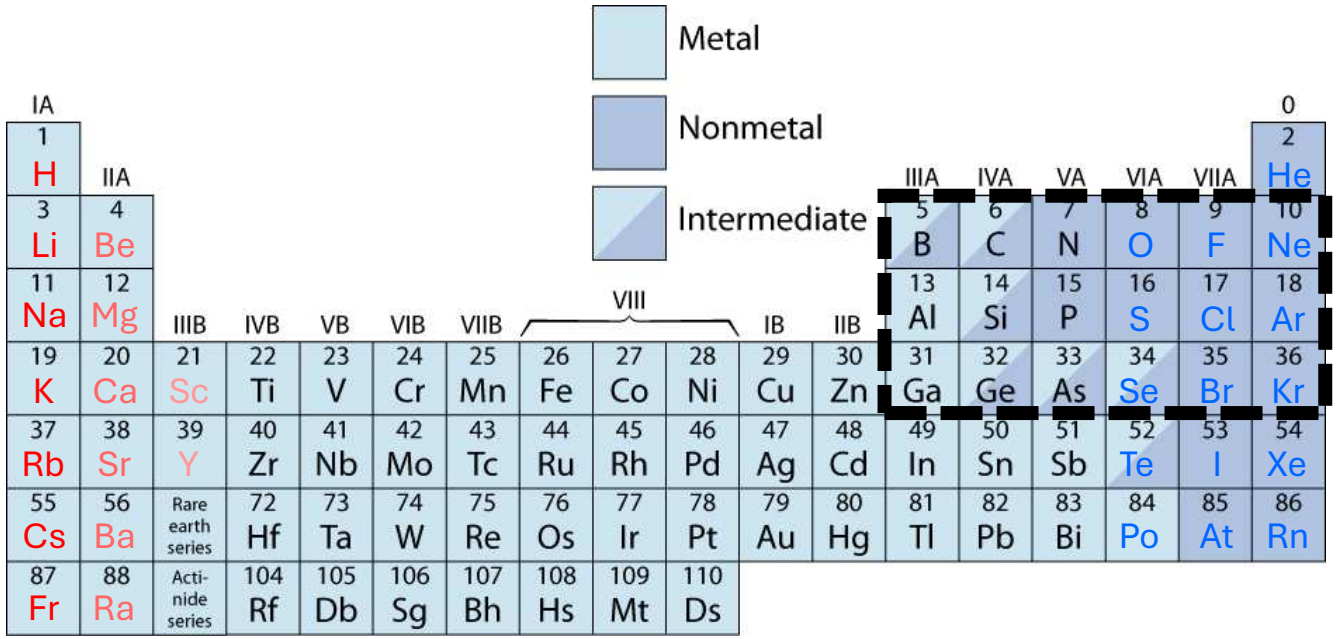


Because these molecular orbitals have certain shapes, covalent bonds are **highly directional!**

...unlike ionic bonds....

Will become important when we discuss structure

Covalent versus *metallic* bonding



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Readily acquire electrons
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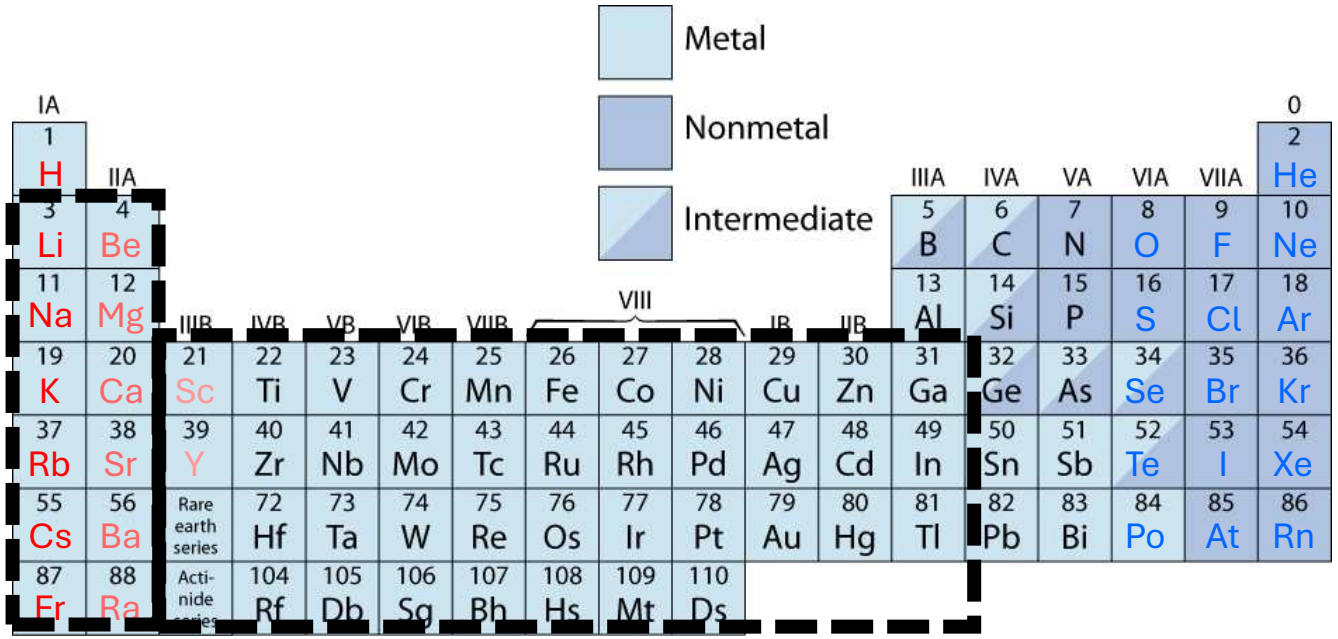
Larger electronegativity

Covalent bonding examples:

- SiC, O_2, GaAs, P_2O_5

Notice these are all between elements that are quite **electronegative** → they really want to *gain* electrons

Covalent versus *metallic* bonding



Electropositive elements:
Readily give up electrons
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Larger electronegativity

Covalent bonding examples:

- SiC, O_2, GaAs, P_2O_5

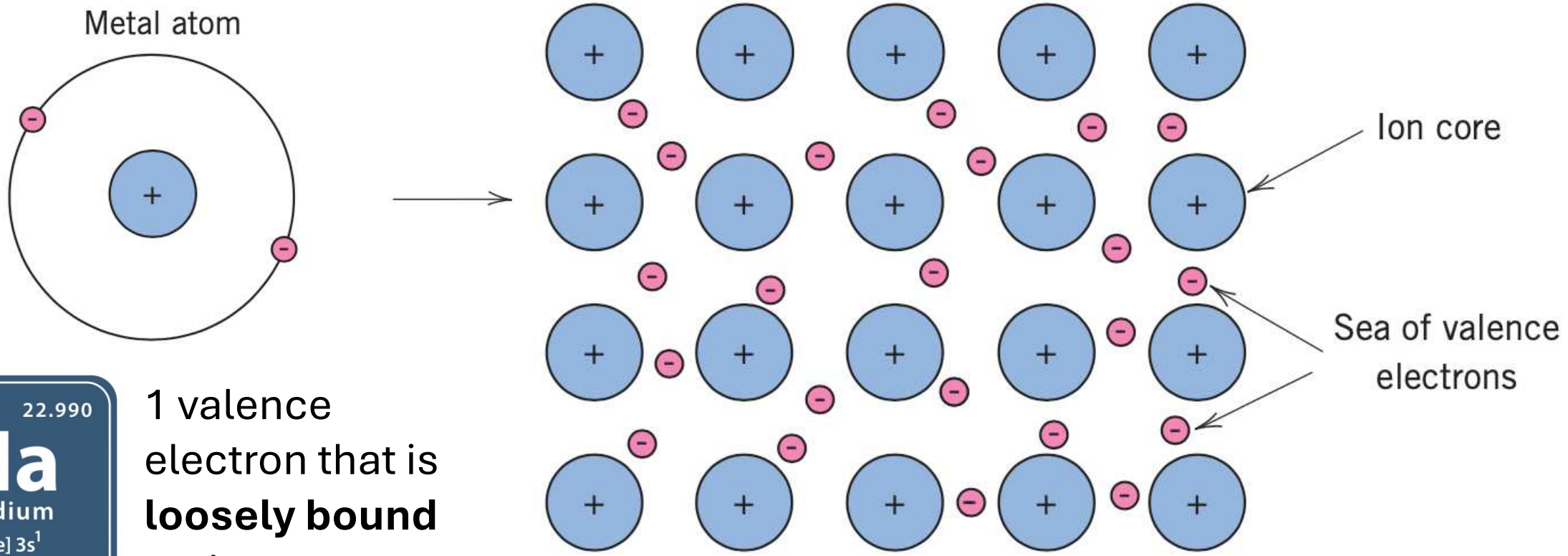
Notice these are all between elements that are quite **electronegative** → they really want to *gain* electrons

How about bonding between **similarly electropositive elements?**

- Na, Mg, Fe, NiTi, FeAl, Cu_2Ni

→ **Form *metallic* bonds**

Metals form a "*sea*" of delocalized electrons





1 valence electron that is **loosely bound** to the atom

When many atoms come together, they **give up their valence electrons to the sea**

This **sea of electrons (negatively charged)** acts as the "glue" which holds together the **(positively charged) ion cores**

Metals form a "*sea*" of delocalized electrons

Because these valence electrons are delocalized, metals are **excellent conductors** of electricity and heat

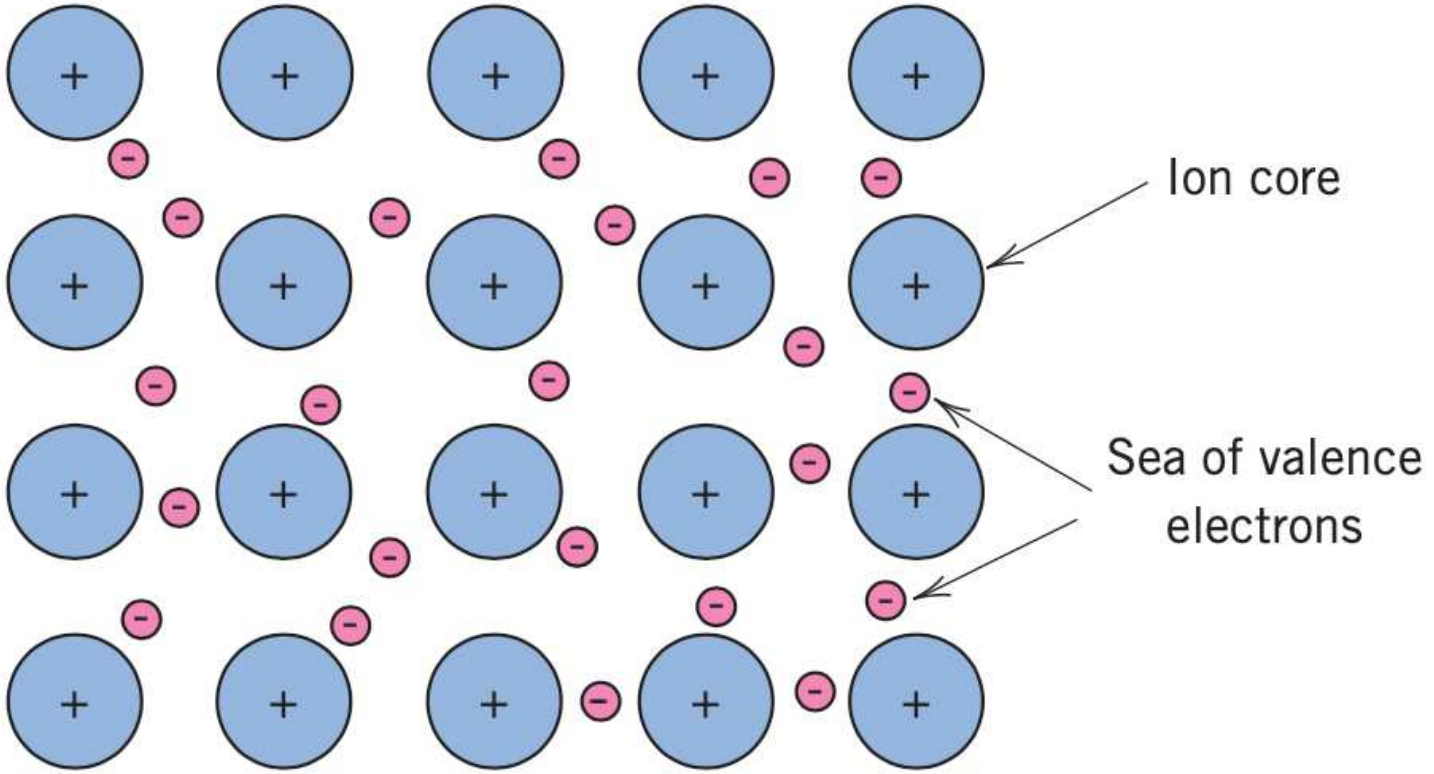
In contrast: **ionic materials are insulating**

(localized charge)

Bonding

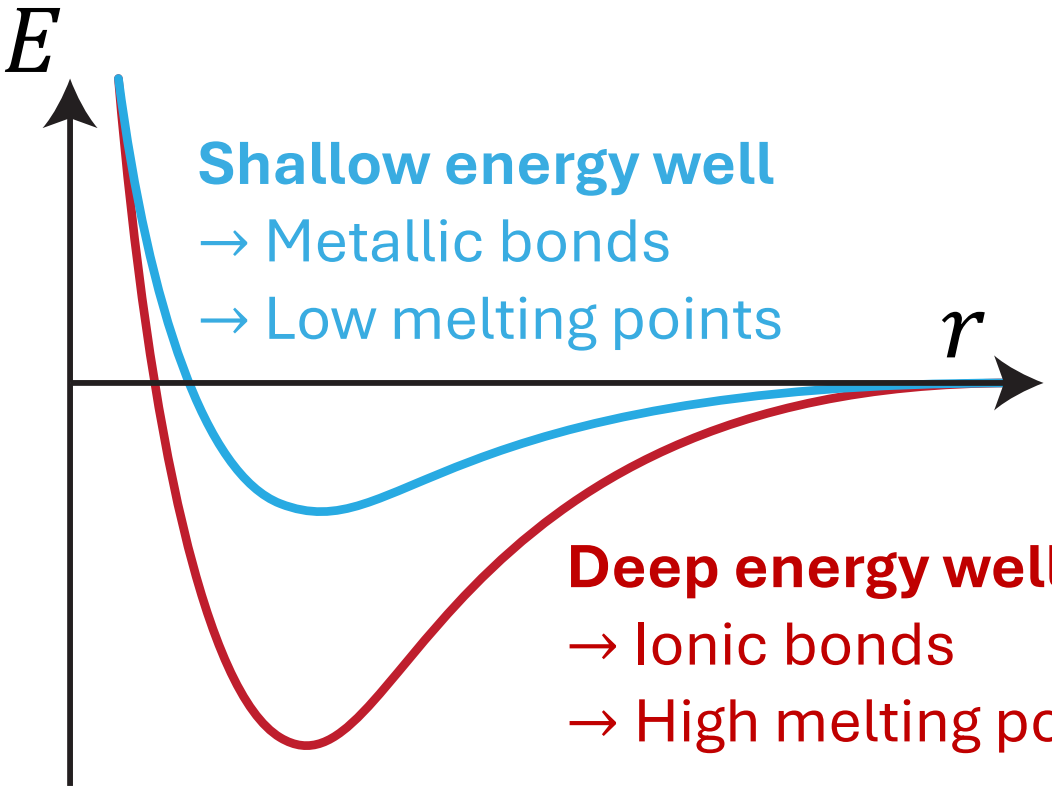
↓ ↑

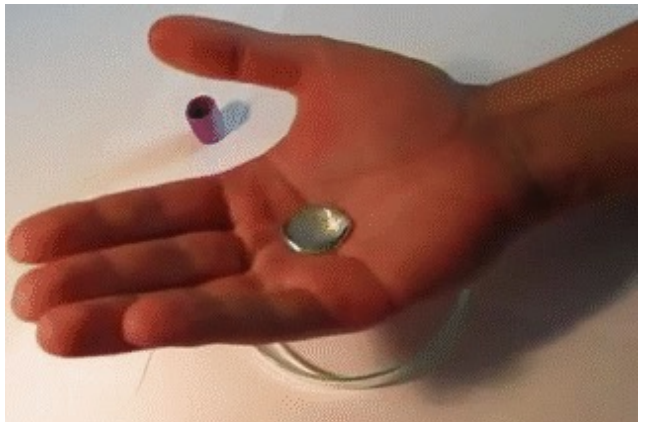
Properties



This **sea of electrons (negatively charged)** acts as the "glue" which holds together the **(positively charged) ion cores**

Bonding ↔ Properties





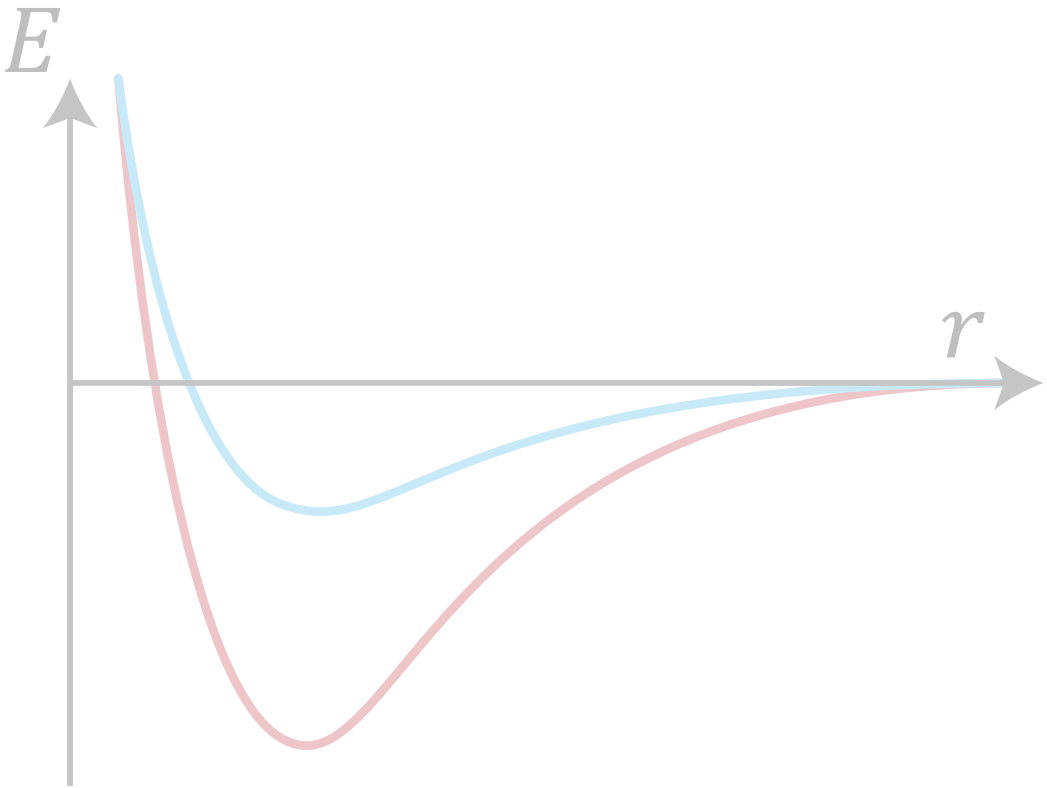
Gallium metal
(T_m ~ 85 °F)

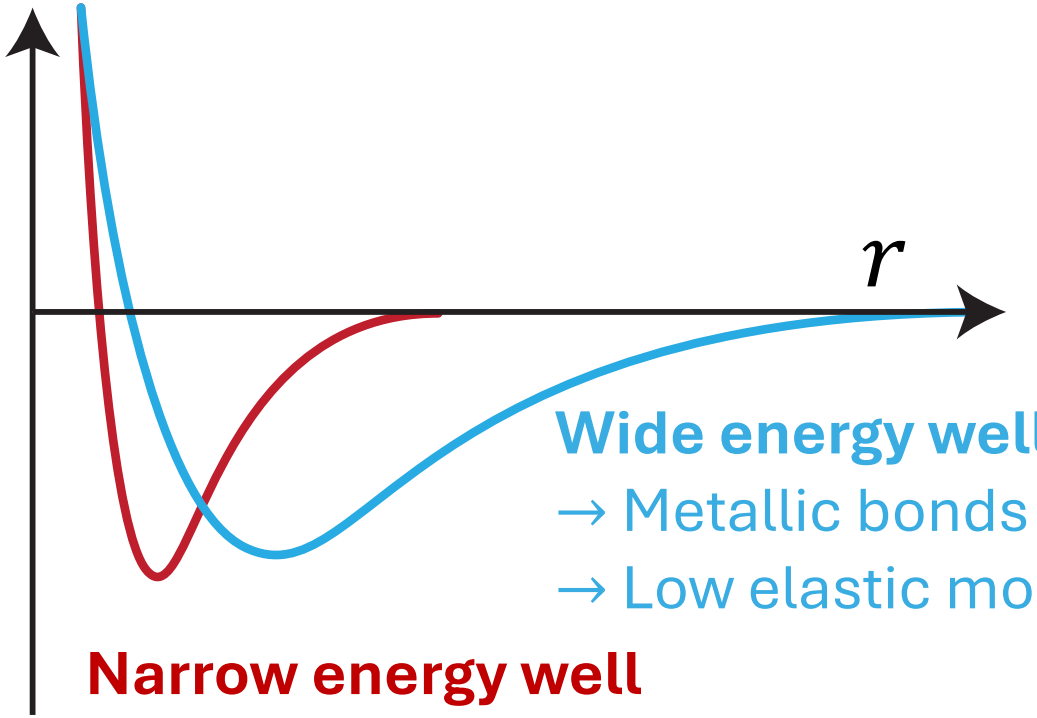


Al_2O_3
(T_m ~ 3700 °F)



Bonding ↔ Properties



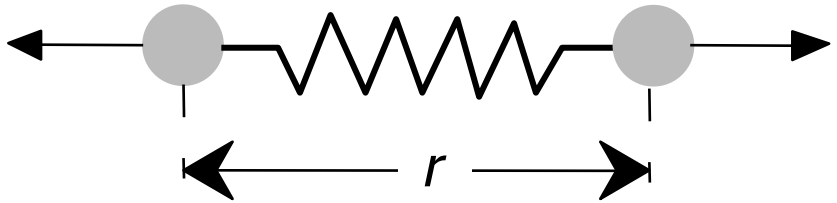


Wide energy well
→ Metallic bonds
→ Low elastic modulus

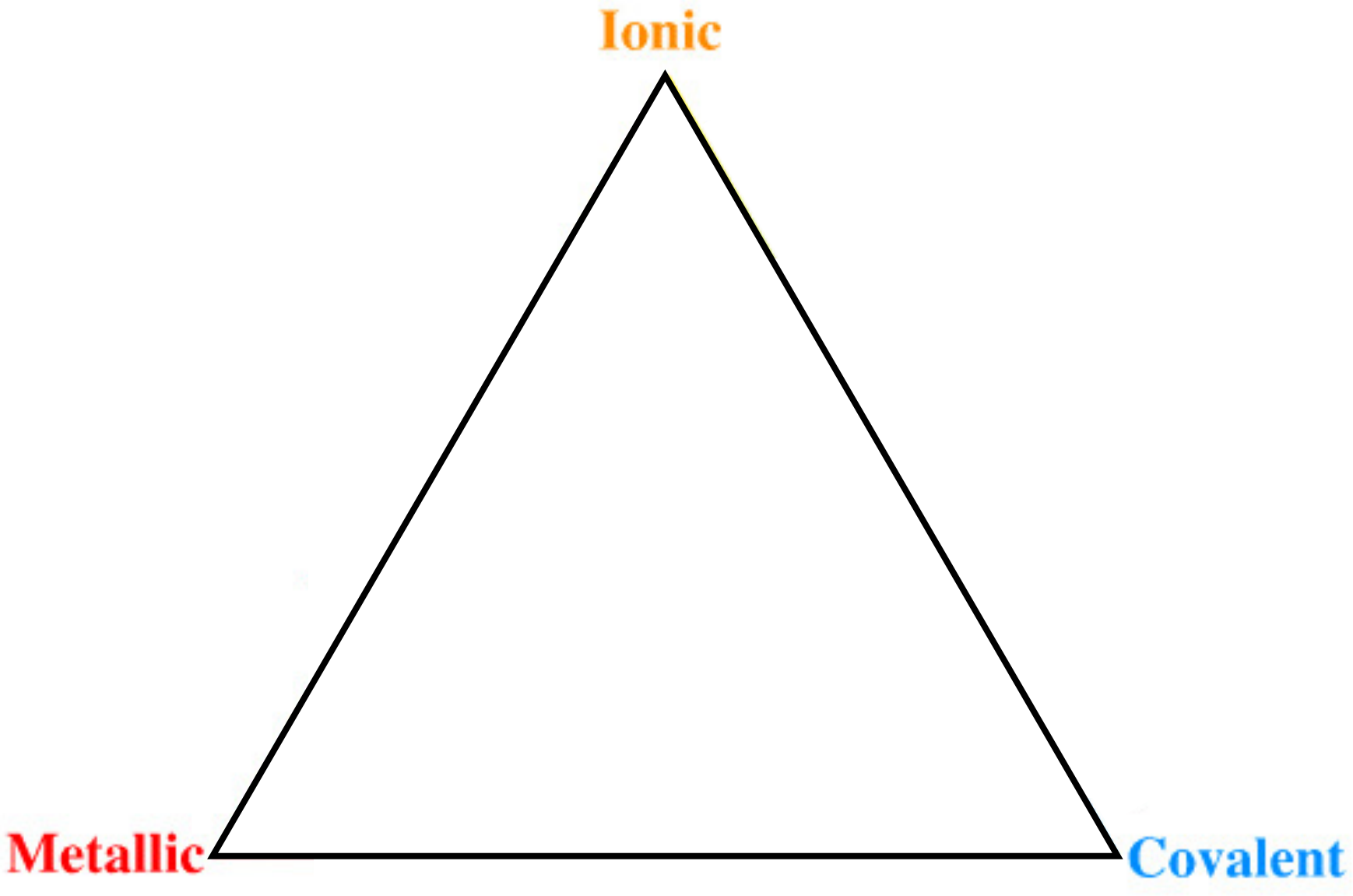
Narrow energy well
→ Ionic/covalent bonds
→ High elastic modulus

Hooke's Law: $F = -kx$

Where $\boldsymbol{k = d^2E/dx^2}$



Most bonds lie somewhere “in the middle”



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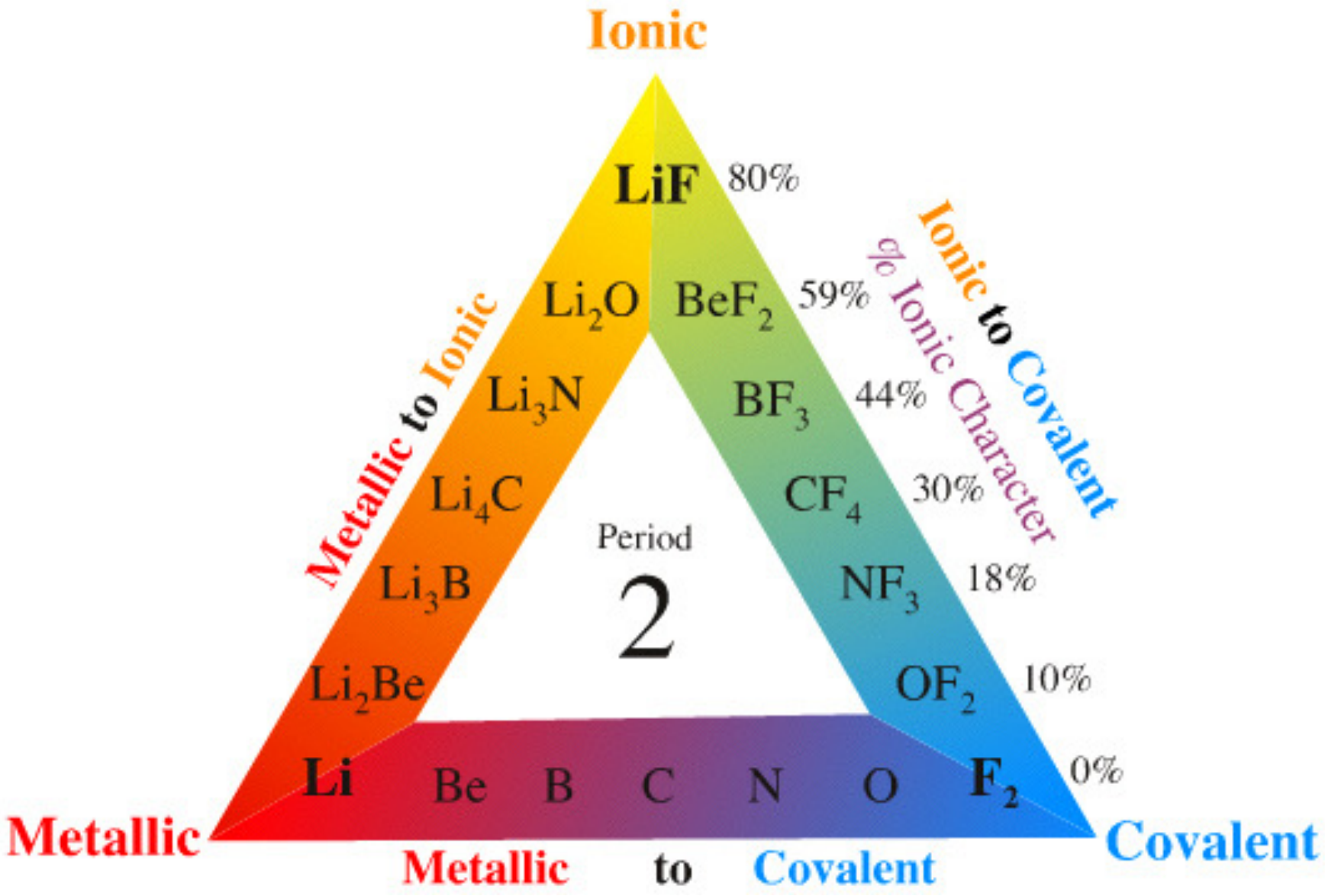
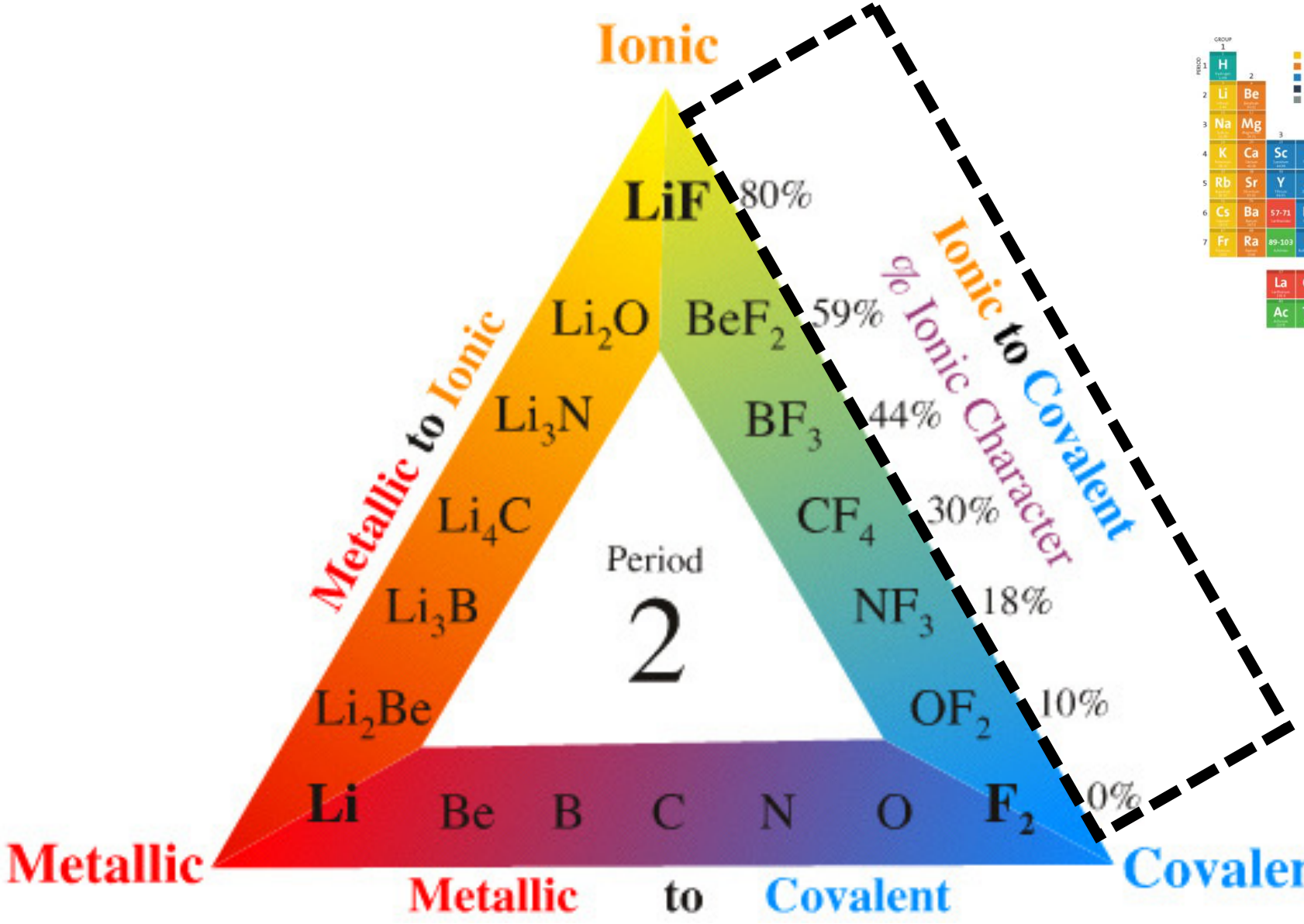
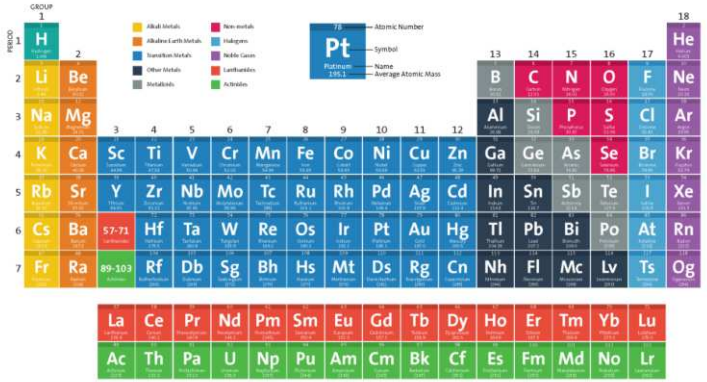


Most bonds lie somewhere “in the middle”

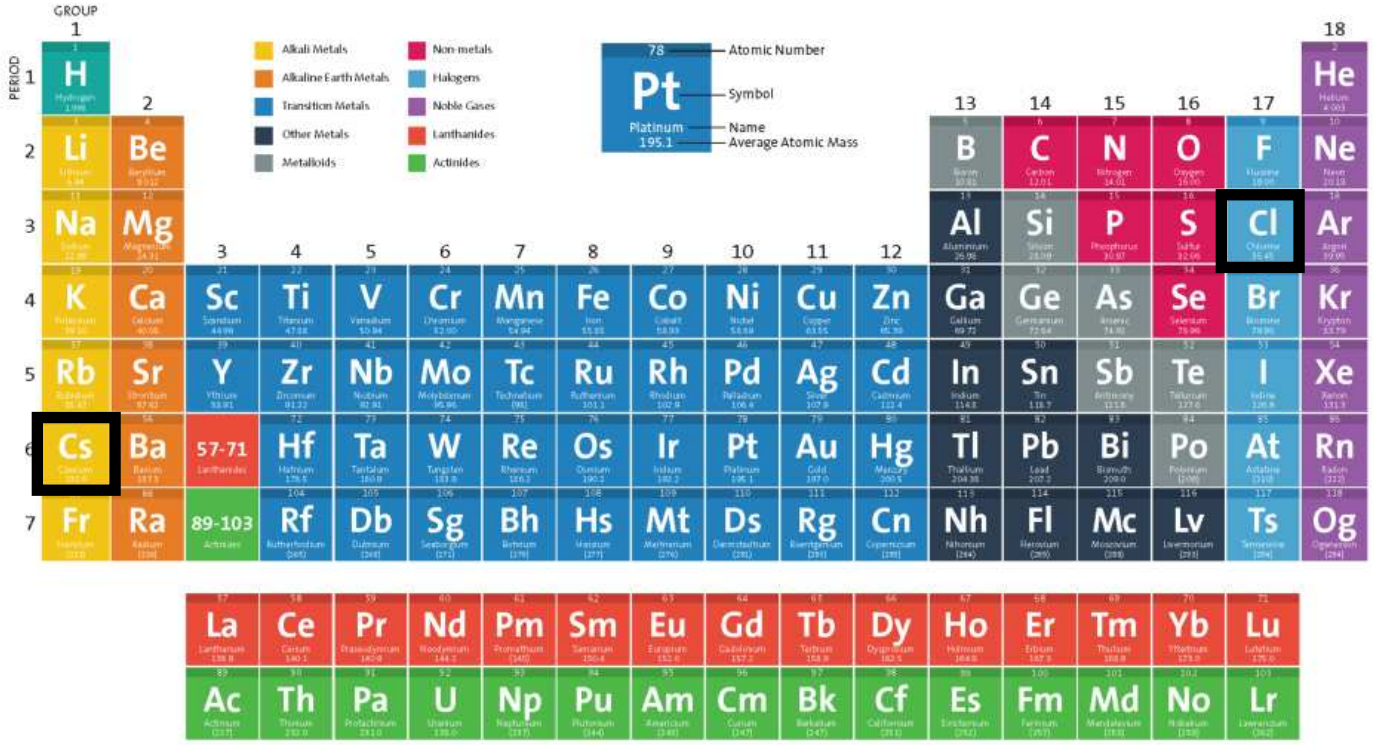




% ionic character is related to the difference in electronegativity – how close elements are on the periodic table

Most bonds lie somewhere “in the middle”

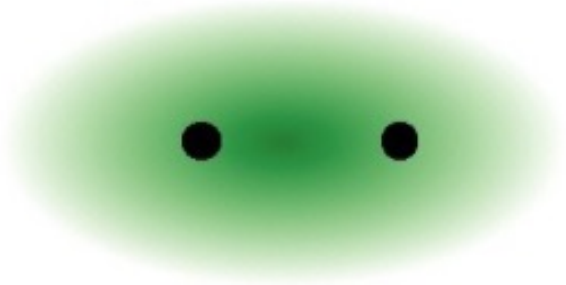
Cs-Cl = **very ionic**

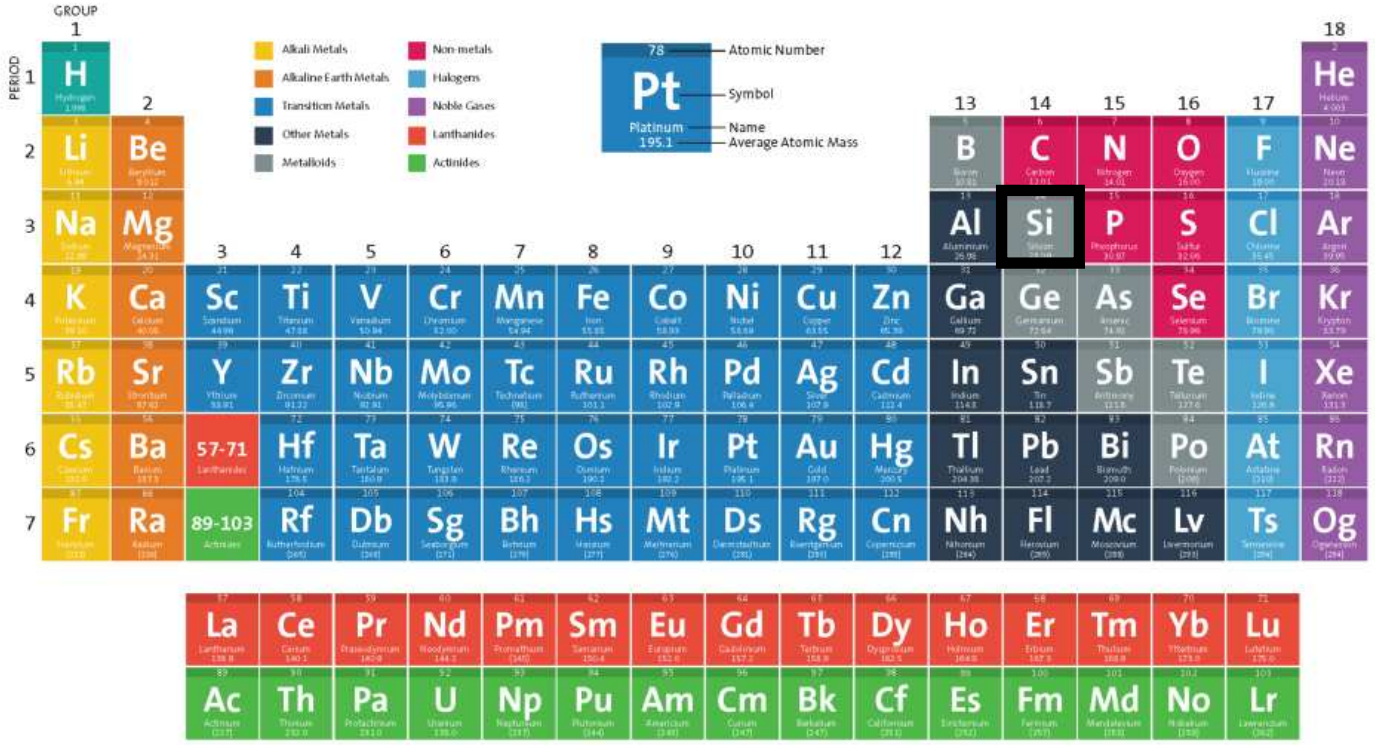


Most bonds lie somewhere “in the middle”

Cs-Cl = **very ionic**

Si-Si = **pure covalent**





Most bonds lie somewhere “in the middle”

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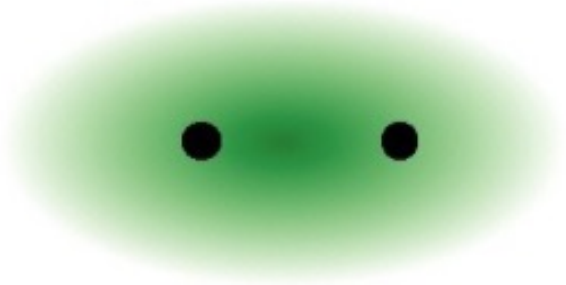
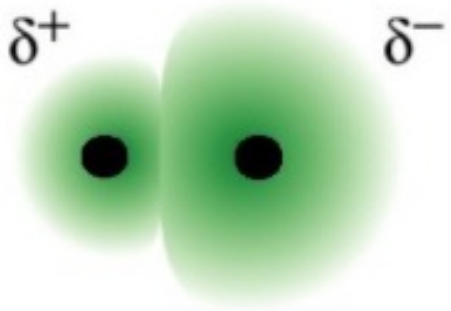
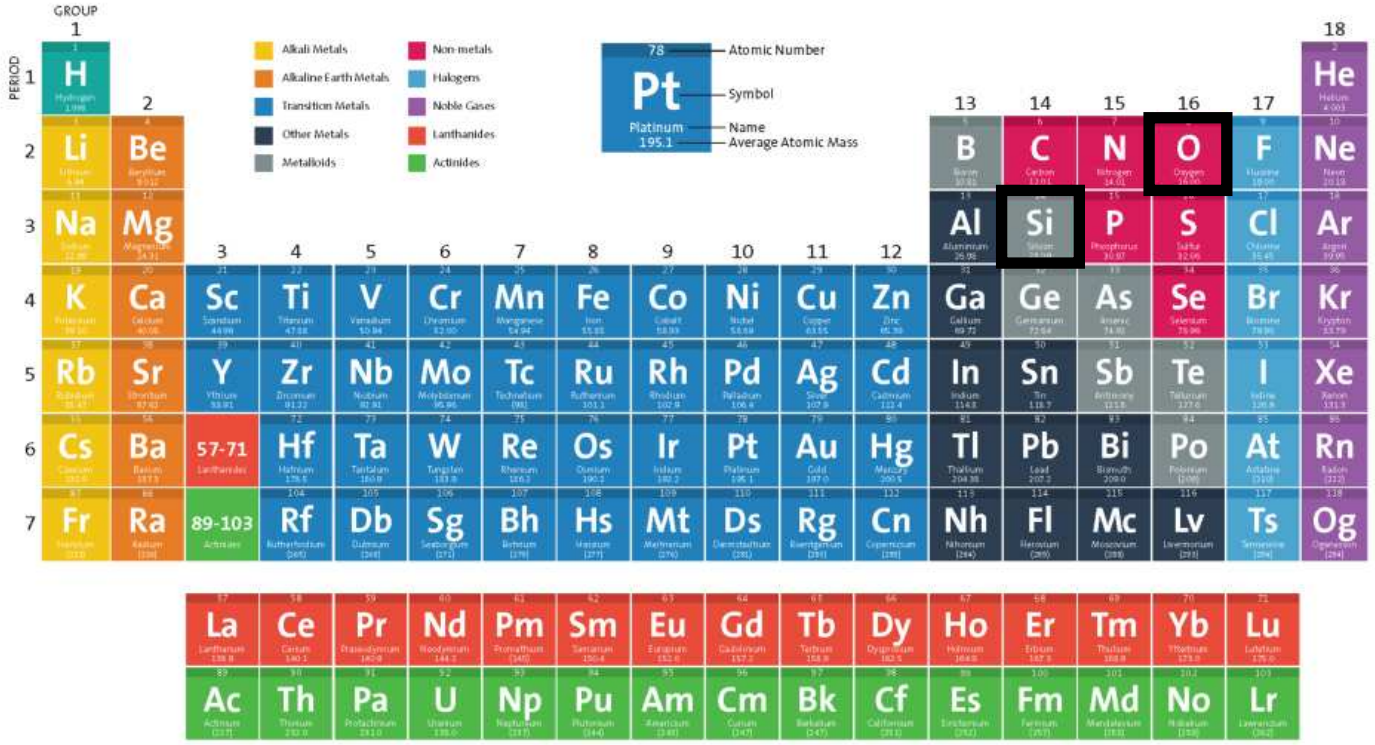


Si-O = **polar covalent**





$$\%\mathrm{IC} = \{1 - \exp[-(0.25)(X_\mathrm{A} - X_\mathrm{B})^2]\} \times 100$$

Electronegativity difference

Example % IC calculations

Cs-Cl = **very ionic**

$$X_{\mathrm{Cs}} = 0.79$$

$$X_{\mathrm{Cl}} = 3.16$$

$$\%\ IC = 100\times\left[1 - e^{-0.25(3.16-0.79)^2}\right] \approx \mathbf{75.4}\%$$

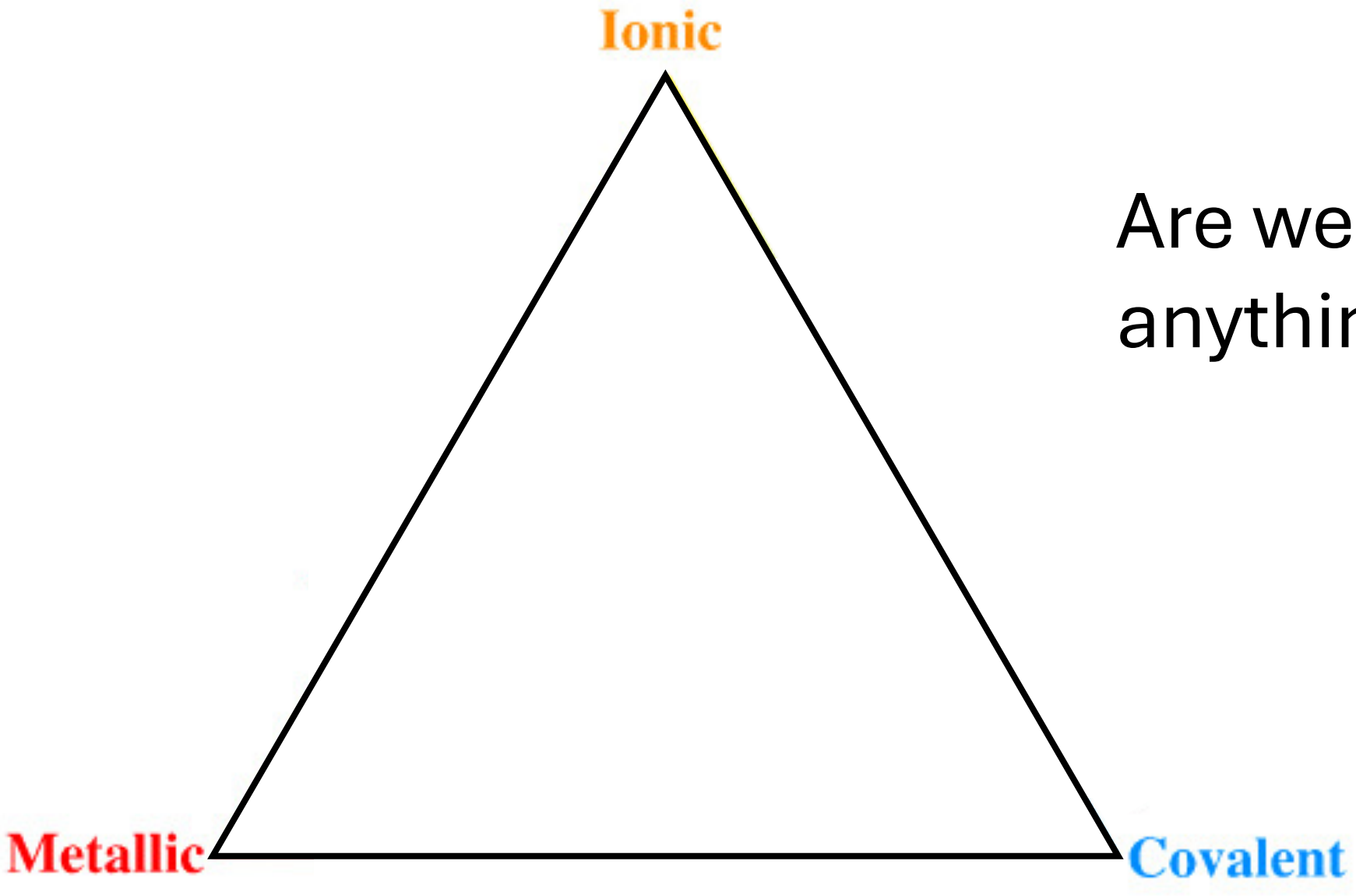
Si-O = **polar covalent**

$$X_{\mathrm{Si}} = 1.90$$

$$X_{\mathrm{O}} = 3.44$$

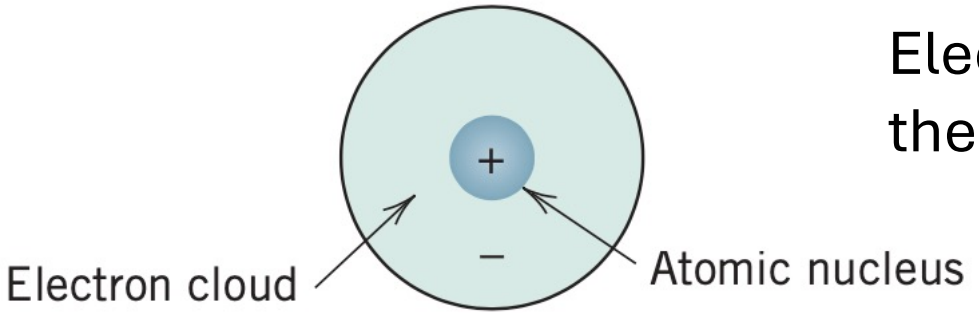
$$\%\ IC = 100\times\left[1 - e^{-0.25(3.44-1.90)^2}\right] \approx \mathbf{44.7}\%$$

Back to our bonding triangle



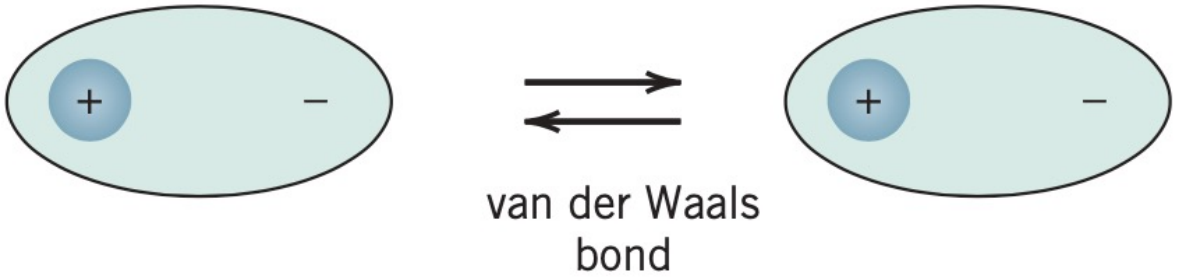
Are we missing anything?

Secondary (van der Waals) bonding

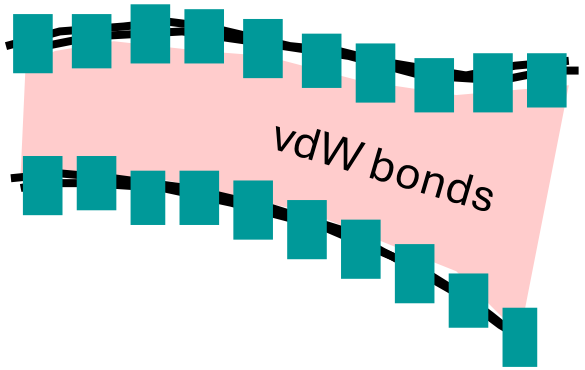


Electron cloud is symmetric about the nucleus → no net dipole

But if we bring two atoms together, they can ***induce* dipoles** in one another, resulting in net attraction



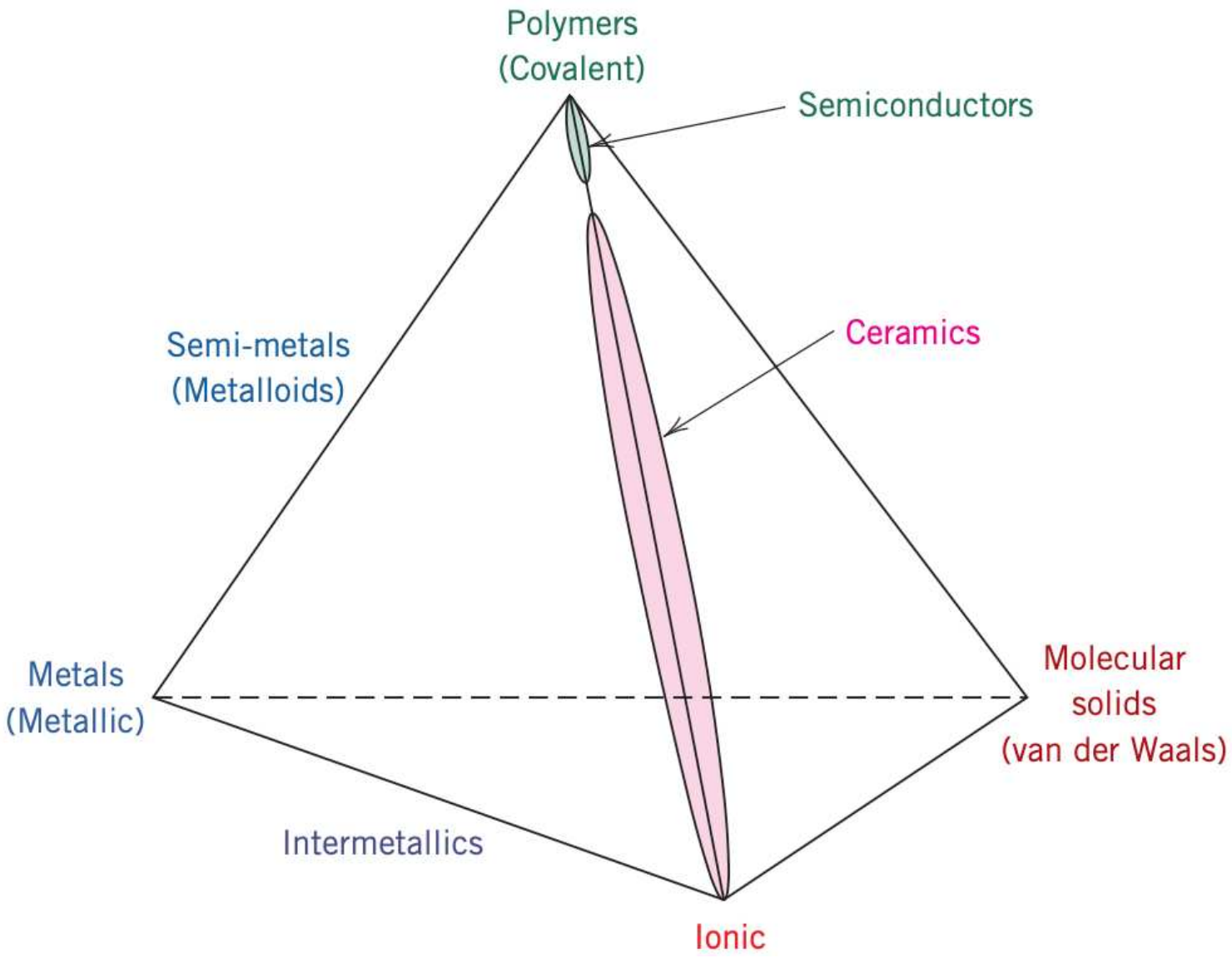
These are generally ***very weak* bonds**



We'll come across them in **polymers**
(think plastic: low T_m)



Summary



Next time:

We'll talk about how bonding dictates **crystal structure**

