

# Chapter 2: Atomic Structure & Interatomic Bonding

## Review...

- Atom and related basics
- Atom electron configuration and valence electrons
- Bonding between atoms and types of bonds in materials



# Class Exercise: Review of Basics for Atom

Includes interactive visualizations, properties, orbitals, isotopes, and compound mixing.

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**Element name & symbol** **Atomic number (Z)** **# of electron in each shell** **(Averaged) Atomic mass (A)**

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 <b>H</b> Hydrogen 1.008	2 <b>He</b> Helium 4.002602	3 <b>Li</b> Lithium 6.94	4 <b>Be</b> Beryllium 9.0121...	5 <b>B</b> Boron 10.81	6 <b>C</b> Carbon 12.011	7 <b>N</b> Nitrogen 14.007	8 <b>O</b> Oxygen 15.999	9 <b>F</b> Fluorine 18.998...	10 <b>Ne</b> Neon 20.1797	11 <b>Na</b> Sodium 22.989...	12 <b>Mg</b> Magnesium 24.305	13 <b>Al</b> Aluminum 26.981...	14 <b>Si</b> Silicon 28.085	15 <b>P</b> Phosphorus 30.973...	16 <b>S</b> Sulfur 32.06	17 <b>Cl</b> Chlorine 35.45	18 <b>Ar</b> Argon 39.948
19 <b>K</b> Potassium 39.0983	20 <b>Ca</b> Calcium 40.078	21 <b>Sc</b> Scandium 44.955...	22 <b>Ti</b> Titanium 47.867	23 <b>V</b> Vanadium 50.9415	24 <b>Cr</b> Chromium 51.9961	25 <b>Mn</b> Manganese 54.938...	26 <b>Fe</b> Iron 55.845	27 <b>Co</b> Cobalt 58.933...	28 <b>Ni</b> Nickel 58.6934	29 <b>Cu</b> Copper 63.546	30 <b>Zn</b> Zinc 65.38	31 <b>Ga</b> Gallium 69.723	32 <b>Ge</b> Germanium 72.63	33 <b>As</b> Arsenic 74.921...	34 <b>Se</b> Selenium 78.971	35 <b>Br</b> Bromine 79.904	36 <b>Kr</b> Krypton 83.798
37 <b>Rb</b> Rubidium 85.4678	38 <b>Sr</b> Strontium 87.62	39 <b>Y</b> Yttrium 88.90584	40 <b>Zr</b> Zirconium 91.224	41 <b>Nb</b> Niobium 92.90637	42 <b>Mo</b> Molybdenum 95.95	43 <b>Tc</b> Technetium (98)	44 <b>Ru</b> Ruthenium 101.07	45 <b>Rh</b> Rhodium 102.90...	46 <b>Pd</b> Palladium 106.42	47 <b>Ag</b> Silver 107.8682	48 <b>Cd</b> Cadmium 112.414	49 <b>In</b> Indium 114.818	50 <b>Sn</b> Tin 118.710	51 <b>Sb</b> Antimony 121.760	52 <b>Te</b> Tellurium 127.60	53 <b>I</b> Iodine 126.90...	54 <b>Xe</b> Xenon 131.293
55 <b>Cs</b> Caesium 132.90...	56 <b>Ba</b> Barium 137.327	57-71 <b>Lanthanoids</b>	72 <b>Hf</b> Hafnium 178.49	73 <b>Ta</b> Tantalum 183.84	74 <b>W</b> Tungsten 186.207	75 <b>Re</b> Rhenium 186.207	76 <b>Os</b> Osmium 190.23	77 <b>Ir</b> Iridium 192.217	78 <b>Pt</b> Platinum 195.084	79 <b>Au</b> Gold 196.96...	80 <b>Hg</b> Mercury 200.59	81 <b>Tl</b> Thallium 204.38	82 <b>Pb</b> Lead 207.2	83 <b>Bi</b> Bismuth 208.98...	84 <b>Po</b> Polonium (209)	85 <b>At</b> Astatine (210)	86 <b>Rn</b> Radon (222)
87 <b>Fr</b> Francium (223)	88 <b>Ra</b> Radium (226)	89-103 <b>Actinoids</b>	104 <b>Rf</b> Rutherfordium (267)	105 <b>Db</b> Dubnium (268)	106 <b>Sg</b> Seaborgium (271)	107 <b>Bh</b> Bohrium (272)	108 <b>Hs</b> Hassium (270)	109 <b>Mt</b> Meitnerium (276)	110 <b>Ds</b> Darmstadtium (281)	111 <b>Rg</b> Roentgenium (280)	112 <b>Cn</b> Copernicium (285)	113 <b>Uut</b> Ununtrium (284)	114 <b>Fl</b> Flerovium (289)	115 <b>Uup</b> Ununpentium (288)	116 <b>Lv</b> Livermorium (293)	117 <b>Uus</b> Ununseptium (294)	118 <b>Uuo</b> Ununoctium (294)

For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.

- Element name? **Carbon**
- Atomic number (Z)? **Z=6**
- # of electrons in a neutral atom? **=Z=6**
- (Averaged) Atomic mass (A) and Unit? **A=12.011 g/mol**
- # protons in such an atom? **=Z=6**



# Atomic Structure

- Atom –
  - electrons (-)  $9.11 \times 10^{-31}$  kg
  - protons
  - neutrons (+) }  $1.67 \times 10^{-27}$  kg
- Atomic number (Z) = # of protons in nucleus of atom  
= # of electrons for a **neutral** atom
- Isotope: same Z, different number of neutrons
- Atomic mass unit (amu), 1/12 mass of  $^{12}\text{C}$
- Atomic mass (or weight) A = averaged mass with respect to natural isotopes for an element

Unit of atomic mass: **g/mol (preferred)** or amu/atom

- 1 mole of atoms: Avogadro number  $N_A = 6.022 \times 10^{23}$  of atoms
- Examples:
  - For C, atomic mass = 12.011 g/mol, i.e., 12.011 g for  $6.022 \times 10^{23}$  of C atoms
  - For H, atomic mass = 1.008 g/mol, i.e., 1.008 g for  $6.022 \times 10^{23}$  of H atoms



# Class Exercise – Periodic Table

Given information on right from periodic table for aluminum,

•What is the atomic number  $Z$

13

•What is the number of proton in Al nucleus

13

•What is the atomic weight  $A$  and the unit for atomic weight  $A$

26.98 g/mol

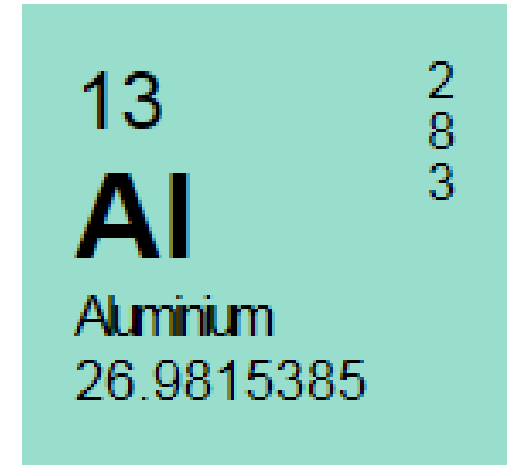
•On average, one gram of Al will contain how many Al atoms?

(Knowing Avogadro's number  $N_A = 6.02 \times 10^{23} \text{ mol}^{-1}$ )

$$\frac{1}{A} \cdot N_A = \frac{1 \text{ g}}{26.98 \text{ g / mol}} \cdot 6.02 \times 10^{23} / \text{mol} = 2.23 \times 10^{22}$$

•What is the averaged (over naturally occurring isotope) mass (weight) for one aluminum atom?

$$4 \quad \frac{A}{N_A} = \frac{26.98 \text{ g / mol}}{6.02 \times 10^{23} / \text{mol}} = 4.48 \times 10^{-23} \text{ g}$$

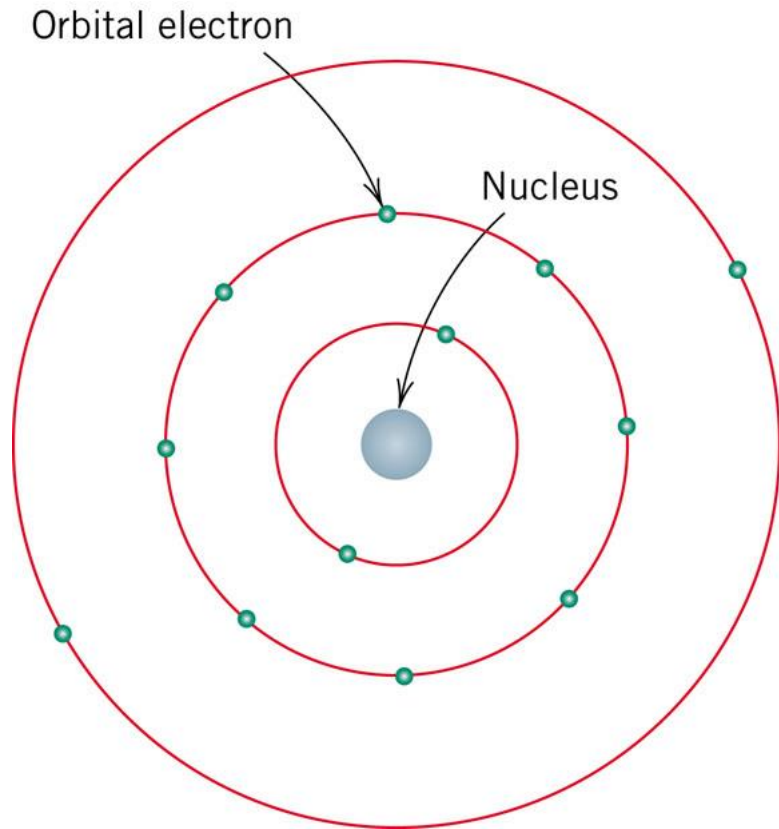


13	2
Al	8
Aluminium	3
26.9815385	

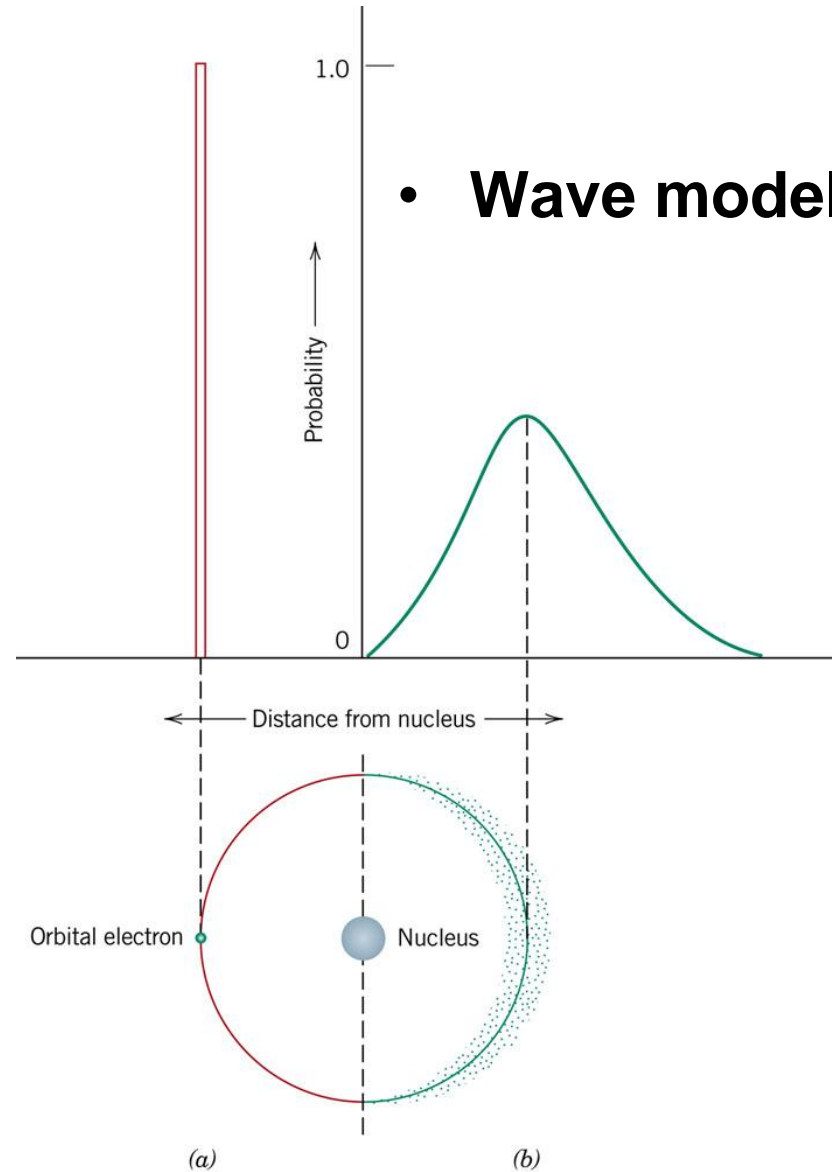


# Atomic (or Electron) Orbital Models

- **Bohr model**



- **Wave model**



# Electronic Structure for Atoms

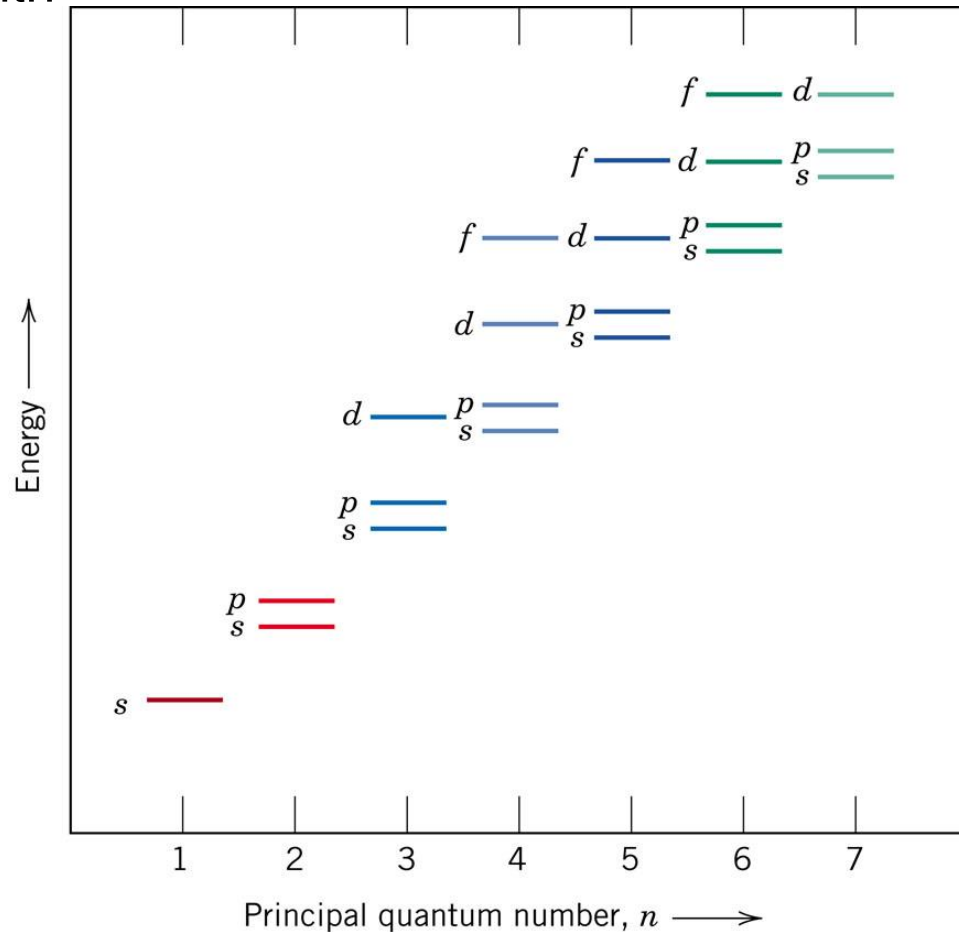
In an atom, electrons have certain arrangement/structure:

- Electrons are in a series of orbitals with different, discrete energy states following certain rules

- Electrons occupy lower available energy states (orbitals) first

- Shell: K, L, M, (or 1, 2, 3) etc. from low to high energy
- Subshell: s, p, d, f, etc. within a shell from low to high energy
- Different orientations (orbits) of same energy within each subshell (for an isolated single atom)

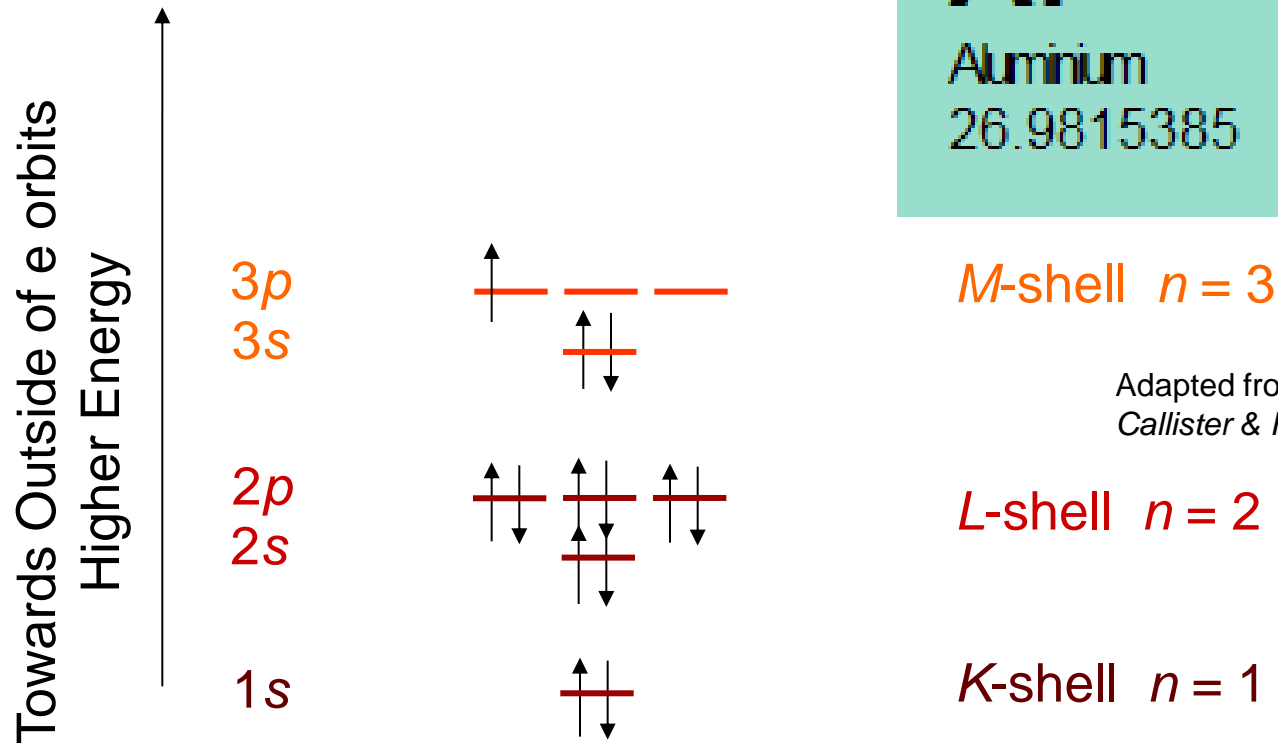
- Follow Pauli exclusion principle: no more than two electrons in the same orbit, with one spin up & one spin down



# Electron Configuration

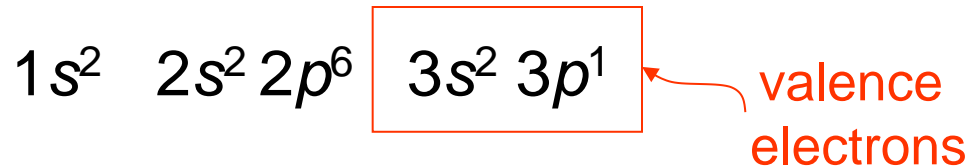
ex: Aluminum, Al - atomic #  $Z = 13$

13	2
<b>Al</b>	8
Aluminium	3
26.9815385	



Adapted from Fig. 2.4,  
*Callister & Rethwisch 8e.*

Electron configuration for a neutral Al atom



# Examples of Electron Configuration

<u>Element</u>	<u>Atomic #</u>	<u>Electron configuration</u>
Hydrogen	1	$1s^1$
Helium	2	$1s^2$ (stable)
Lithium	3	$1s^2 2s^1$
Beryllium	4	$1s^2 2s^2$
Boron	5	$1s^2 2s^2 2p^1$
Carbon	6	$1s^2 2s^2 2p^2$
...	...	...
Neon	10	$1s^2 2s^2 2p^6$ (stable)
Sodium	11	$1s^2 2s^2 2p^6 3s^1$
Magnesium	12	$1s^2 2s^2 2p^6 3s^2$
Aluminum	13	$1s^2 2s^2 2p^6 3s^2 3p^1$
...	...	...
Argon	18	$1s^2 2s^2 2p^6 3s^2 3p^6$ (stable)
...	...	...
Krypton	36	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$ (stable)

Adapted from Table 2.2,  
Callister & Rethwisch 8e.





# Valence Electrons

- **Valence electrons** – those electrons occupy outmost **shells** (and, for transition metals, a few of of inner shell electrons in the d-orbits)
  - Valence electrons are most available for bonding and tend to control the chemical properties for the atom/element
- example: Neutral Cl atom - atomic number  $Z = 17$



valence electrons

- Valence electrons determine the following properties
  - 1) Chemical
  - 2) Electrical
  - 3) Thermal
  - 4) Optical
- **Atoms/ions with filled outmost shell will be stable:**  
For H, He, Li, Be: two(2) e<sup>-</sup> for 1s as the outmost shell is stable  
For others: outmost shell with eight (8) e<sup>-</sup> is stable





# Electronegativity

- A number representing the tendency for an atom to **acquire** electrons
- Right side of periodic table & fewer number of shells → **HIGHER** electronegativity, easier to GET electron(s)
- Left side of periodic table & more number of shells → **LOWER** electronegativity, easier to GIVE OUT electron(s)

IA	IIA		III A - VIII										VIA - VIIA					0
H 2.1													B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	He -
Li 1.0	Be 1.5												Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	Ne -
Na 0.9	Mg 1.2		IIIB	IVB	VB	VIB	VII B	VIII			IB	IIB	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Ar -
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	Xe -	
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2	Rn -	
Cs 0.7	Ba 0.9	La-Lu 1.1-1.2	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Po 2.0	At 2.2	Rn -				
Fr 0.7	Ra 0.9	Ac-No 1.1-1.7																

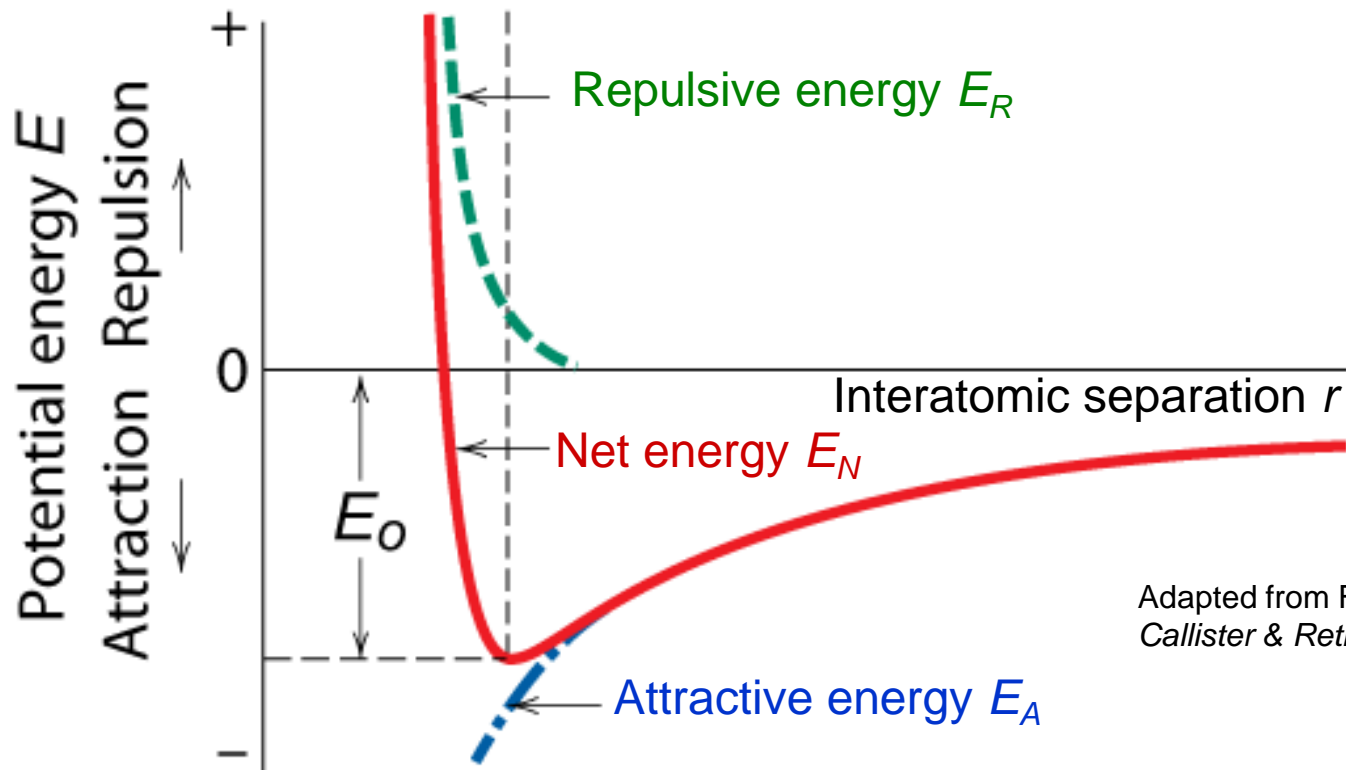
**LOWER** electronegativity

**HIGHER** electronegativity



# Bonding Energy

- In materials, atoms are bonded together in certain ways
- Bonding energy - energy required to **break** the bonds between atoms
- Result of balance of **attractive** and **repulsive** forces
  - minimum energy  $\rightarrow$  most stable  $\rightarrow$  stable inter-atomic distance

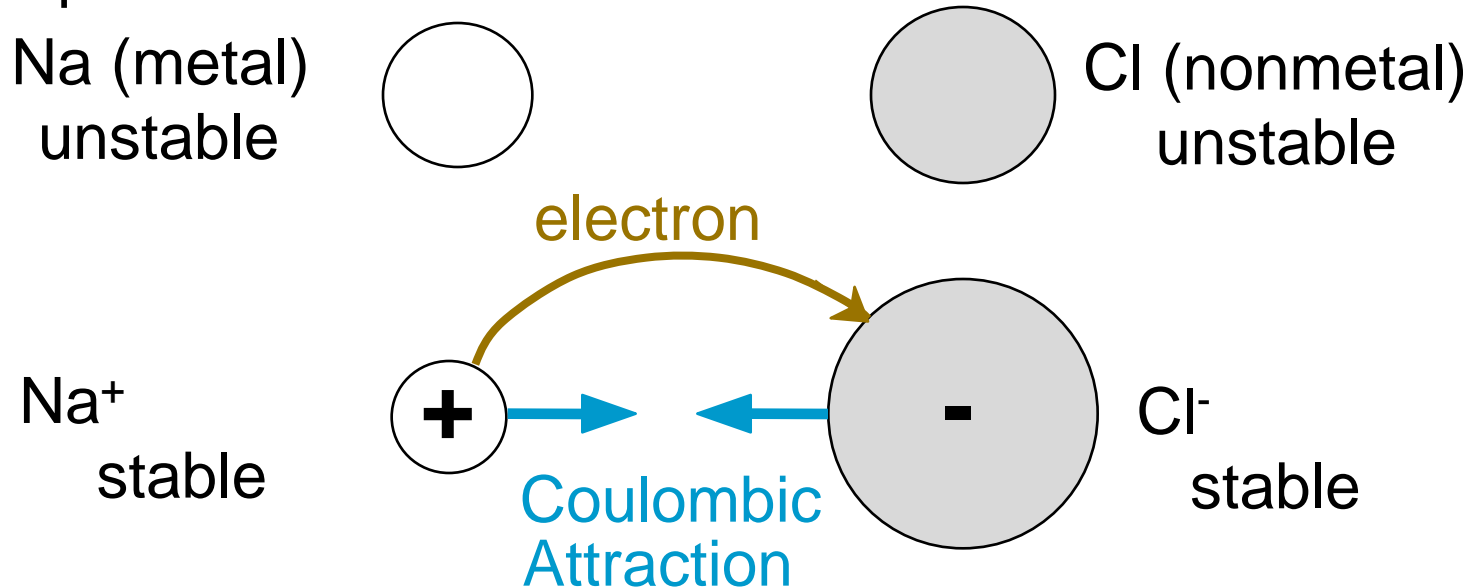


Adapted from Fig. 2.8(b),  
Callister & Rethwisch 8e.



# Primary Bond (1) - Ionic Bond

- Occurs between + and - ions.
- Requires **electron transfer between atoms**.
- Large difference in electronegativity between bonded atoms required.
- Example: NaCl

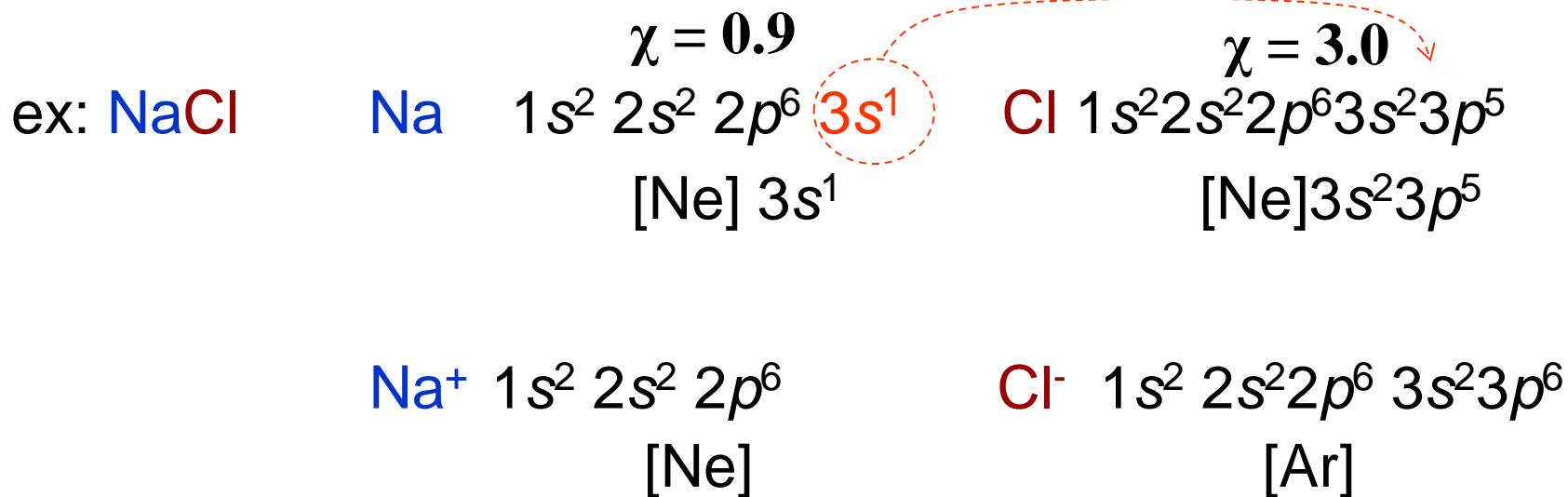


- Large bond energy

Ionic bond – metal + nonmetal

↑  
donates  
electrons

↑  
accepts  
electrons



# Examples: Ionic Bond

- Often found in **Ceramics**

The periodic table below shows electronegativity values for various elements. Arrows indicate the formation of ionic compounds from these elements:

- NaCl**: Sodium (Na, 0.9) and Chlorine (Cl, 3.0)
- MgO**: Magnesium (Mg, 1.2) and Oxygen (O, 3.5)
- CaF<sub>2</sub>**: Calcium (Ca, 1.0) and Fluorine (F, 4.0)
- CsCl**: Cesium (Cs, 0.7) and Chlorine (Cl, 3.0)

IA																	0	
H																	He	
2.1	IIA											IIIA	IVA	VA	0	VIA	VIIA	
Li	Be											B	C	N	O	F	Ne	
1.0	1.5											2.0	2.5	3.0	3.5	4.0	-	
Na	Mg											Al	Si	P	S	Cl	Ar	
0.9	1.2											1.5	1.8	2.1	2.5	3.0	-	
		IIIB	IVB	VB	VIB	VII B	VIII				IB	IIB						
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
0.8	1.0	1.3	1.5	1.6	1.6	1.5	1.8	1.8	1.8	1.9	1.6	1.6	1.8	2.0	2.4	2.8	-	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
0.8	1.0	1.2	1.4	1.6	1.8	1.9	2.2	2.2	2.2	1.9	1.7	1.7	1.8	1.9	2.1	2.5	-	
Cs	Ba	La-Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
0.7	0.9	1.1-1.2	1.3	1.5	1.7	1.9	2.2	2.2	2.2	2.4	1.9	1.8	1.8	1.9	2.0	2.2	-	
Fr	Ra	Ac-No																
0.7	0.9	1.1-1.7																

  
Give up electrons

  
Acquire electrons

Adapted from Fig. 2.7, Callister & Rethwisch 8e. (Fig. 2.7 is adapted from Linus Pauling, *The Nature of the Chemical Bond*, 3rd edition, Copyright 1939 and 1940, 3rd edition. Copyright 1960 by Cornell University.



# Primary Bond (2) - Covalent Bond

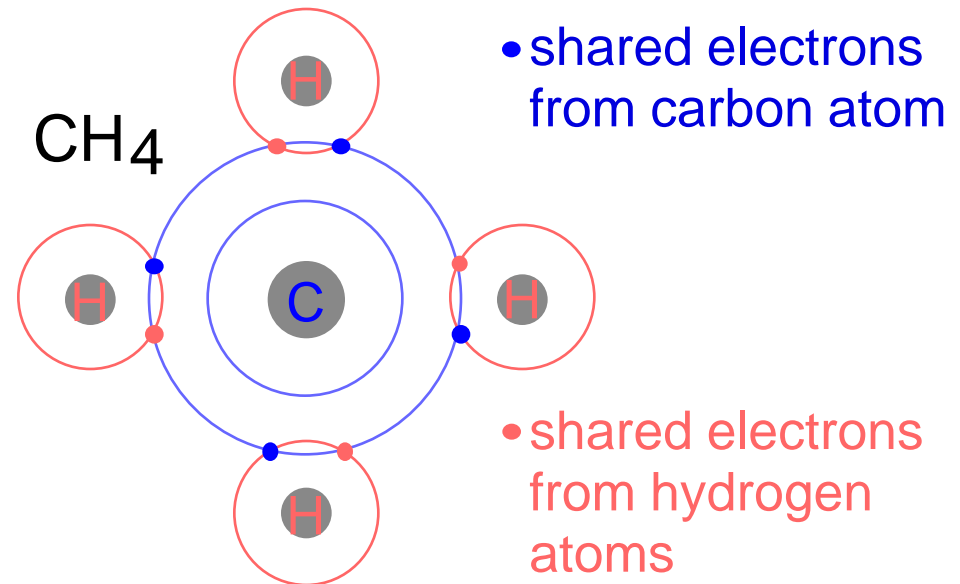
- Between non-metals with similar **electronegativity** → share electrons
- Bonds determined by valence – often *s* & *p* orbitals dominate bonding
- Example: CH<sub>4</sub>

C: has 4 valence e<sup>-</sup>, needs 4 more to be stable

H: has 1 valence e<sup>-</sup>, needs 1 more to be stable

Electronegativities  $\chi$  are **comparable**:

2.1 for H and 2.5 for C



Adapted from Fig. 2.10, *Callister & Rethwisch 8e.*

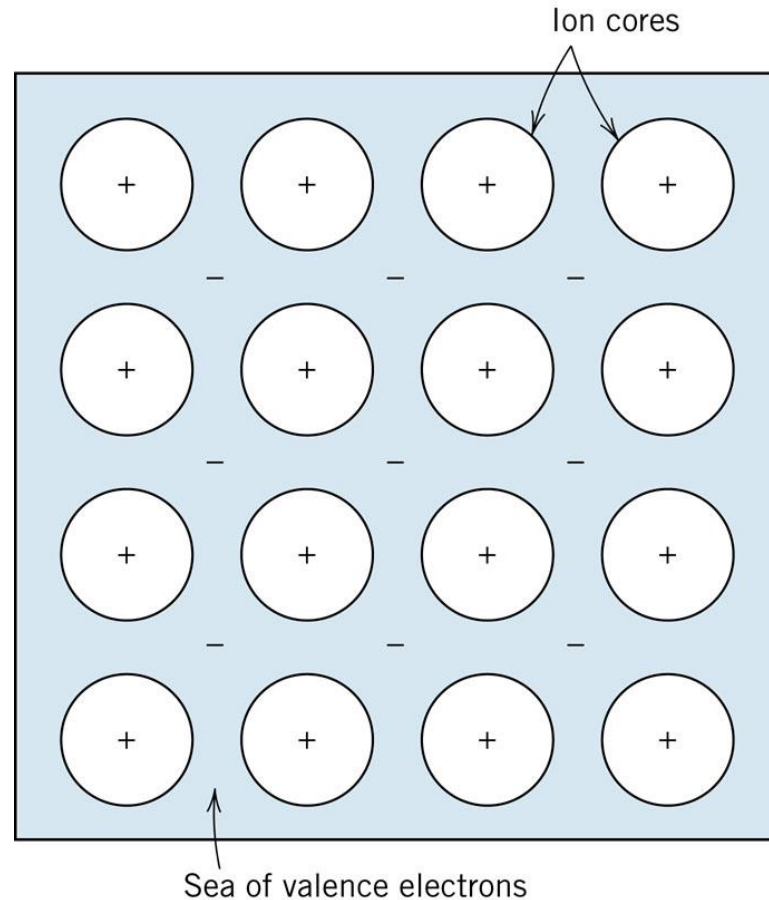
- Bond energy: usually large





# Primary Bond (3) - Metallic Bond

- **Metallic Bond** -- Bonds between metal cations and **delocalized** electron cloud

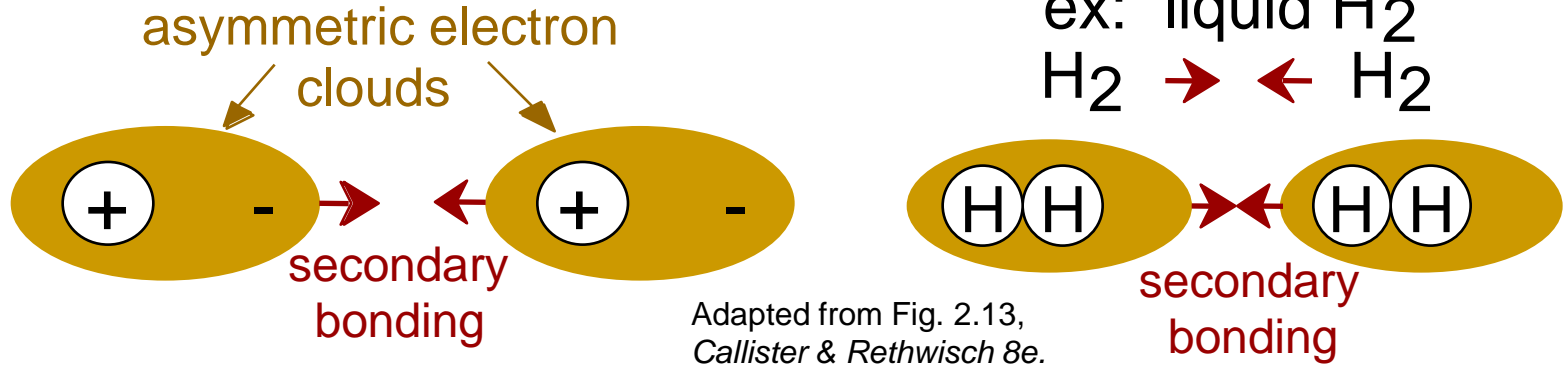


- Bond energy usually large

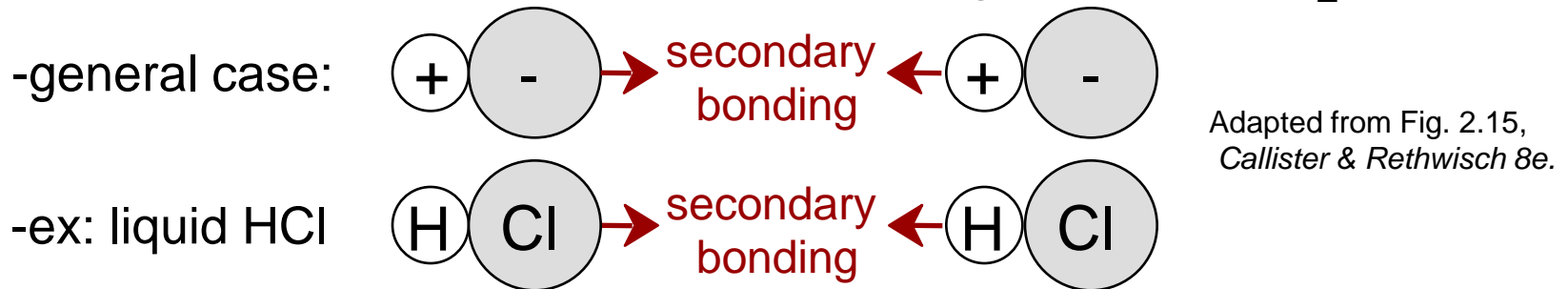
# Secondary Bonds

“Bond” arising from interactions between dipoles in molecules

Case 1: Between fluctuating (induced) dipoles (e.g., for H<sub>2</sub>, Cl<sub>2</sub>)



Case 2: Between permanent dipoles (e.g., for HCl, H<sub>2</sub>O)

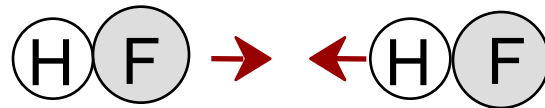


secondary bonding between individual polymer molecules



# Hydrogen Bond – A Special Type of Secondary Bond

- Strongest among all secondary bonds
- A special case of permanent dipole induced bonding
- **Between individual molecules** in which H is covalently bonded to F (e.g., HF), O (e.g., H<sub>2</sub>O), and N (e.g., NH<sub>3</sub>)



- Hydrogen bond bonding energy is much higher than other types of secondary bonding but still much weaker than bonding energy for primary bonds (i.e., covalent, ionic, or metallic bonds)



# Summary: Bond Type (1)

<u>Type</u>	<u>Bonding Energy</u>
<b><u>Primary</u></b> bonds	Ionic Large
	Covalent Variable Large-Diamond Small-Bismuth
	Metallic Variable Large-Tungsten Small-Mercury
<b><u>Secondary</u></b> bonds (between molecules or even particles) e.g., hydrogen bond	Generally small



# Bond Type & Materials Physical Properties

**Table 2.3** Bonding Energies and Melting Temperatures for Various Substances

<i>Bonding Type</i>	<i>Substance</i>	<i>Bonding Energy</i>		<i>Melting Temperature (°C)</i>
		<i>kJ/mol</i>	<i>eV/Atom, Ion, Molecule</i>	
Ionic	NaCl	640	3.3	801
	MgO	1000	5.2	2800
Covalent	Si	450	4.7	1410
	C (diamond)	713	7.4	>3550
Metallic	Hg	68	0.7	-39
	Al	324	3.4	660
	Fe	406	4.2	1538
	W	849	8.8	3410
van der Waals	Ar	7.7	0.08	-189
	Cl <sub>2</sub>	31	0.32	-101
Hydrogen	NH <sub>3</sub>	35	0.36	-78
	H <sub>2</sub> O	51	0.52	0

- Higher bonding energy → Higher melting point



# Materials Class & Bonding Type

## Ceramics

Ionic & covalent bonding

Generally large bonding energy

High  $T_m$

High  $E$  (*Elastic modulus, see Chapter 6*)

## Metals

Metallic bonding

Generally large bonding energy

High  $T_m$

High  $E$

## Polymers

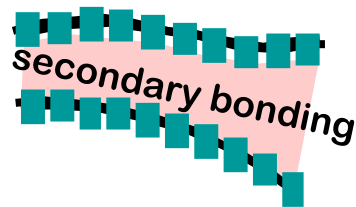
Covalent/secondary bond

Generally low bonding energy

- Secondary bonds dominate interaction between molecules

small  $T_m$

small  $E$



# Class Exercise - Bonds

- Given the following electronegativity numbers
  - $\chi(\text{Na})=0.9$ ;
  - $\chi(\text{F})=4.0$ ;
  - $\chi(\text{Si})=1.8$ ;
  - $\chi(\text{C})=2.5$ ;
  - $\chi(\text{Mg})=1.2$ ;

Determine the predominant primary bond type in the follow materials

- Sodium fluoride (NaF) **Ionic bond**
- Silicon carbide (SiC) **Covalent bond**
- Pure magnesium (Mg) **Metallic bond**



# Class Exercise – Bonds (2)

- What is the bonding type between Oxygen and Oxygen atoms WITHIN a single oxygen molecule?

Covalent bond

- Is the bonding between different oxygen molecules in liquid oxygen primary bonding or secondary bonding?

Secondary bond

- What is the bonding type between Hydrogen (H) and oxygen WITHIN a single water molecule?

Covalent bond

- What is the bonding type BETWEEN different water molecules in ice?

Secondary bond (Hydrogen bond, in particular)





# Class Exercise

Given information on right from periodic table for sodium,

•What is the atomic number  $Z$

11

•What is the number of proton in Na nucleus

11

•What is the atomic weight  $A$  and the unit for atomic weight  $A$

22.99 g/mol

•On average, one gram of Na will contain how many Na atoms?

$1\text{g}/(22.99\text{ g/mol}) \times (6.02 \times 10^{23}/\text{mol}) = 2.62 \times 10^{22}$

•What is the averaged (over naturally occurring isotope) mass (weight) for one sodium atom?

$(22.99\text{ g/mol}) / (6.02 \times 10^{23}/\text{mol}) = 3.82 \times 10^{-23}\text{ g}$

•Knowing F has electron configuration of  $1s^2 2s^2 2p^5$  and atomic weight of 19.0, give the chemical formula for the stable compounds between Na and F and calculate the mass for one mole of that compound

Na has 1 valence e ( $[\text{Ne}]3s^1$ ), F has 7 valence e ( $[\text{Ne}]2s^2 2p^5$ )

One Na atom gives one e to one F atom, both become stable  $\rightarrow \text{NaF}$

Mass for one mole of NaF:  $19.0\text{g} + 23.0\text{g} = 42.0\text{ g}$

The image shows a yellow square representing the periodic table entry for Sodium (Na). In the top left corner is the atomic number 11. In the top right corner are the shell numbers 2, 8, and 1 stacked vertically. In the center is the element symbol 'Na' in a large, bold font. Below the symbol, the word 'Sodium' is written in a smaller font, and at the bottom is the atomic weight '22.98976928'.



# Chapter 2 homework

- Read chapter 2 and give an honor statement confirm reading
- Calister 8ed, hw 2.7, 2.22, and one additional problem



- Calister 8ed, 2.7

*Give the electron configurations for the following ions:  $Fe^{2+}$ ,  $Al^{3+}$ ,  $Cu^+$ ,  $Ba^{2+}$ ,  $Br$ , and  $O^{2-}$ .*

- Calister 8ed, 2.22

*What type(s) of bonding would be expected for each of the following materials: brass (a copper-zinc alloy), rubber, barium sulfide ( $BaS$ ), solid xenon, bronze, nylon, and aluminum phosphide ( $AlP$ )?*

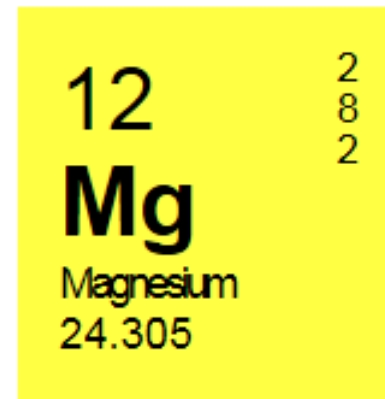
- One additional problem see attached



# Homework

Given information on right from periodic table for magnesium,

- What is the atomic number  $Z$
- What is the number of proton in Mg nucleus
- What is the atomic weight  $A$  and the unit for atomic weight  $A$
- On average, one gram of Mg will contain how many Mg atoms?
- What is the averaged (over naturally occurring isotope) mass (weight) for one magnesium atom?
- Knowing F has electron configuration of  $1s^2 2s^2 2p^5$  and atomic weight of 19.0, give the chemical formula for the stable compounds between Mg and F and calculate the mass for one mole of that compound



12	2 8 2
<b>Mg</b>	
Magnesium	
24.305	

