Materials Science A244
Week 1: Introduction to Materials Science

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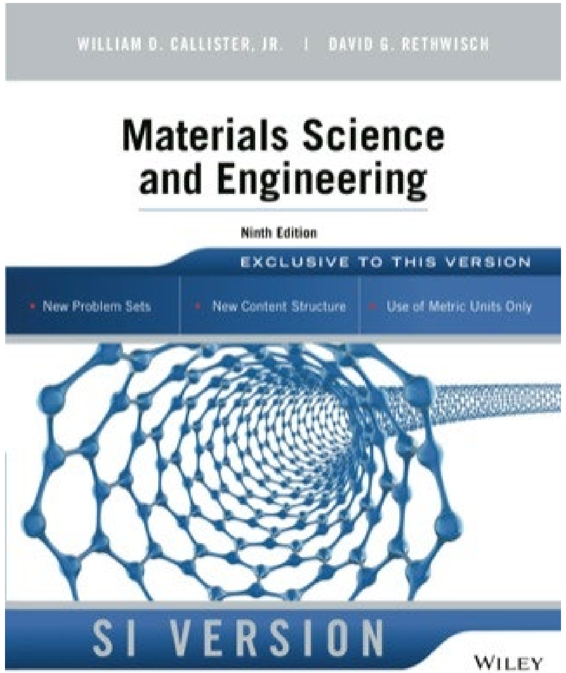
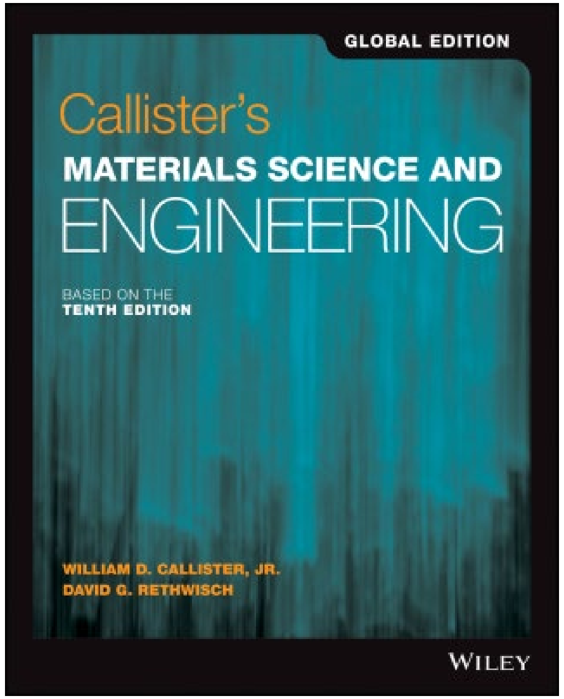


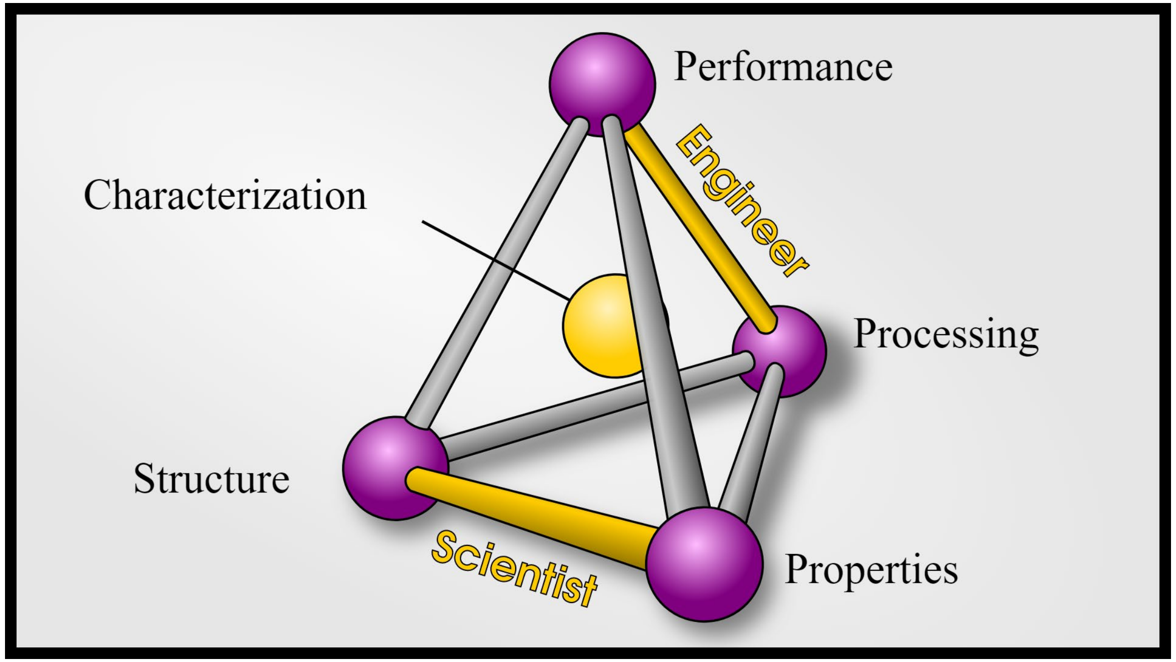
Callister 9th & 10th edition chapters
1: Introduction ♦ 2: Atomic Bonding



Prof Deborah Blaine
Mechanical & Mechatronics Engineering

Materials Science & Engineering Tetrahedron

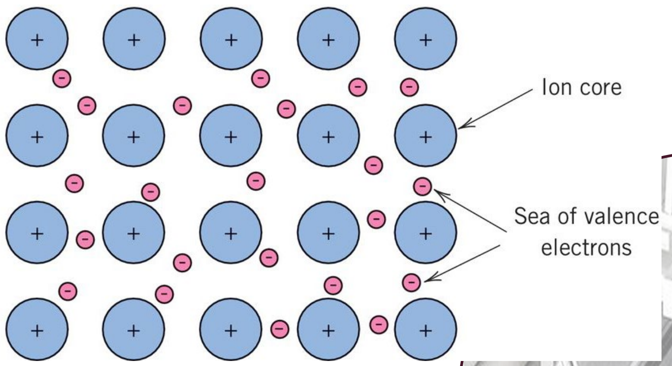
Why are we studying this!?

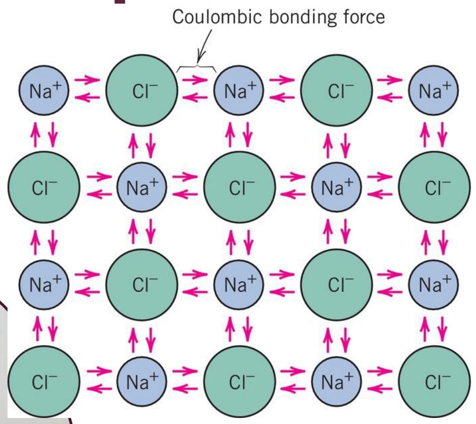


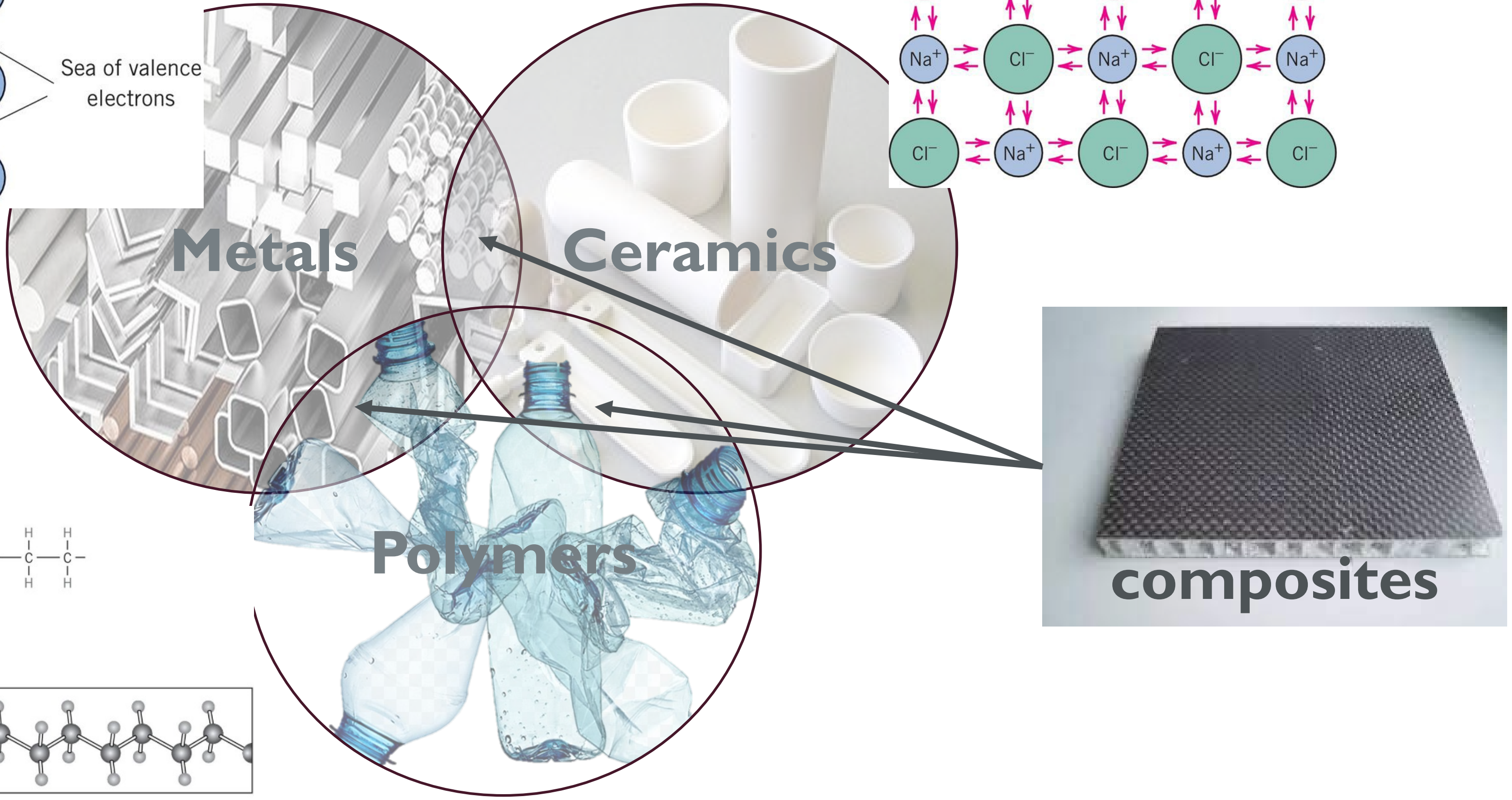
Source: https://msestudent.com/what-is-materials-science-tetrahedron-paradigm/

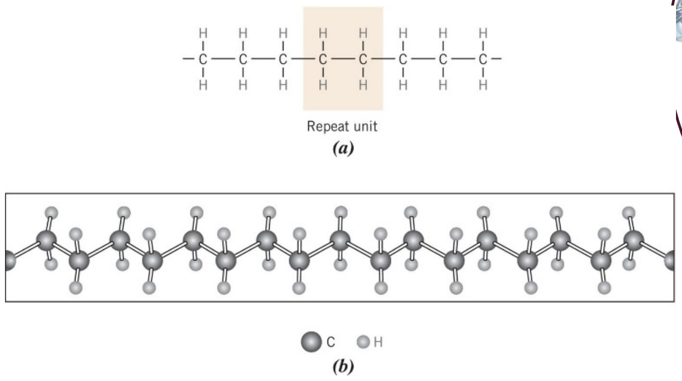
- A materials scientist focuses on the structure of materials in order to create materials with specific properties.
- Engineers create designs that need to meet specific performance requirements. They need to select the correct materials and processes for making the components of their design, so that the material properties are appropriate for the components' function.
- We need to be able to characterise materials in order to determine whether they are fit for purpose, or to design new materials, using new processes that produce materials with properties that meet our required performance characteristics.

Engineering materials: primary groups









Atoms and interatomic bonding

Revision
Eng Chem 123

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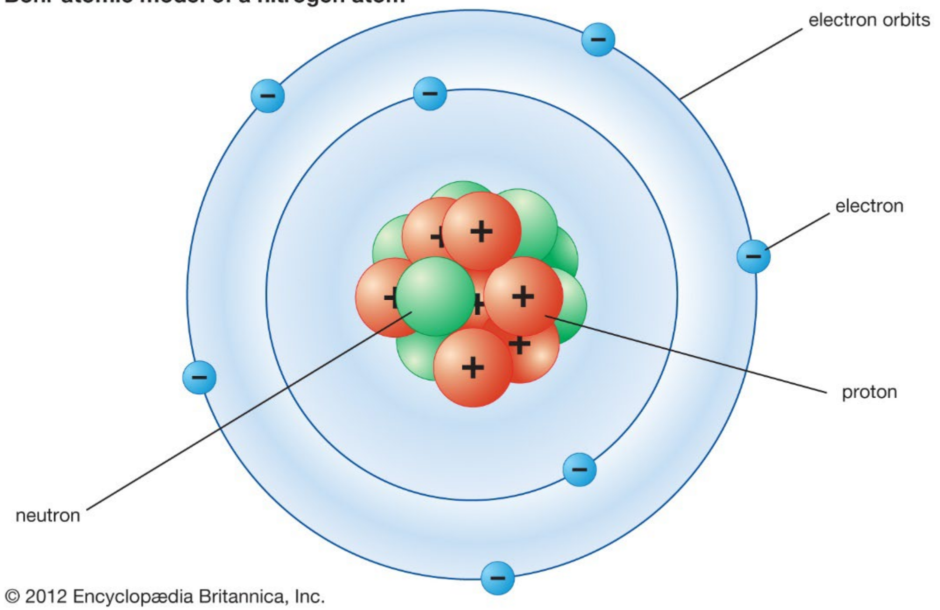
Bohr's atomic model (1913)

- Each atom has a nucleus made up of neutrons and protons with electrons orbiting the nucleus.
- Each chemical element is characterised by its **atomic number, Z,** equal to the number of protons in the nucleus.
- The **atomic mass, A,** of an element is equal to the sum of the masses of protons and neutrons in the nucleus.
- While the number of protons is set for a given element, the number of neutrons can vary, leading to different atomic masses for the same element – these are called **isotopes**.
- The atomic weight, $\bar{A}$, is the weighted average of all the atomic masses of the different isotopes of an element. The atomic mass unit, **amu**, is the mass of 1/12th of a carbon-12 atom and is used to calculated atomic weight.

Bohr atomic model of a nitrogen atom

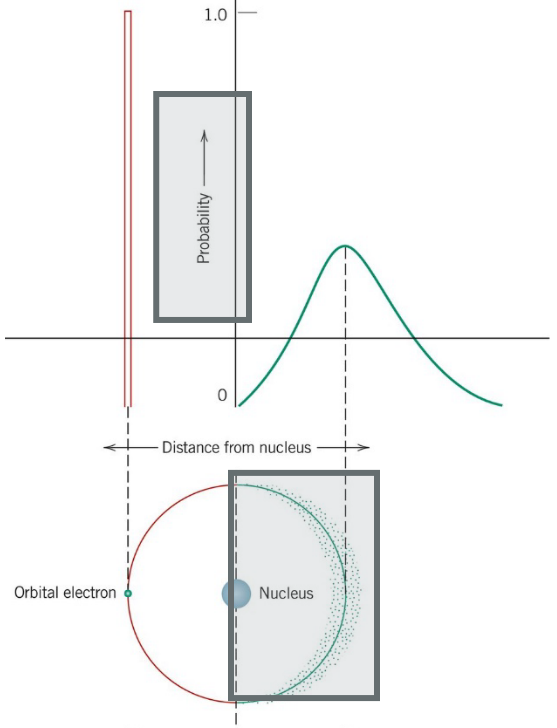


Callister 2.2

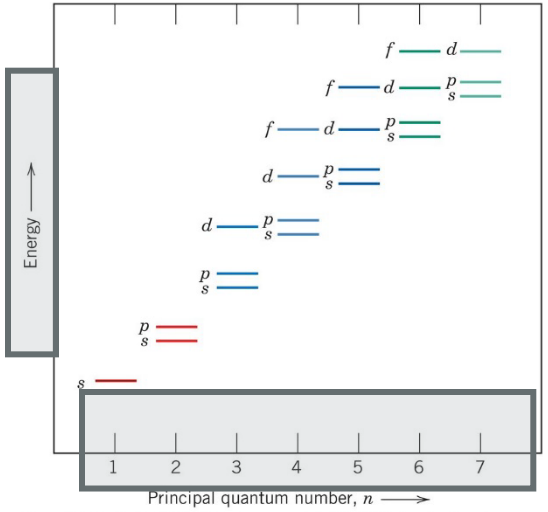
Atoms and Interatomic bonding

Beyond Bohr – wave mechanics and quantum numbers

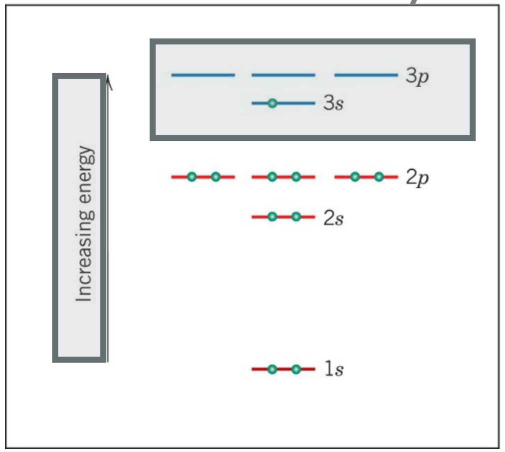
- Expands Bohr's limited atomic model by assuming electrons have both **wave and particle characteristics**, and that the **energy of electrons** can be **quantised** (have a value that can be measured).
- The size, shape and spatial orientation of an electron's probability density (orbital) are characterised by **quantum numbers**.
- The **energy levels** in the electron shells and subshells are characterised by quantum numbers.
- **Valence electrons** occupy the outermost shell and are important as the determine how atoms bond with each other



Adapted from Z. D. Jastrzebski, The Nature and Properties of Engineering Materials, 3rd edition, p. 4. Copyright © 1987 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.



From K. M. Ralls, T. H. Courtney, and J. Wulff, Introduction to Materials Science and Engineering, p. 22. Copyright © 1976 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.



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The periodic table

atomic information on all elements

Electropositive elements

- Easily give up valence electrons
- Become positively charged, e.g.

$$Ba \rightarrow Ba^{2+} + 2e^{-}$$

Key

29	Atomic number
Cu	Symbol
63.55	Atomic weight

Metal

Nonmetal

Intermediate

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII			IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
1 H 1.0080																	2 He 4.0026
3 Li 6.941	4 Be 9.0122											5 B 10.811	6 C 12.011	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.180
11 Na 22.990	12 Mg 24.305											13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.064	17 Cl 35.453	18 Ar 39.948
19 K 39.098	20 Ca 40.08	21 Sc 44.956	22 Ti 47.87	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.845	27 Co 58.933	28 Ni 58.69	29 Cu 63.55	30 Zn 65.41	31 Ga 69.72	32 Ge 72.64	33 As 74.922	34 Se 78.96	35 Br 79.904	36 Kr 83.80
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.4	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.76	52 Te 127.60	53 I 126.90	54 Xe 131.30
55 Cs 132.91	56 Ba 137.33	Rare earth series	72 Hf 178.49	73 Ta 180.95	74 W 183.84	75 Re 186.2	76 Os 190.23	77 Ir 192.2	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.19	83 Bi 208.98	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	Acti-nide series	104 Rf (261)	105 Db (262)	106 Sg (266)	107 Bh (264)	108 Hs (277)	109 Mt (268)	110 Ds (281)								

Rare earth series	57 La 138.91	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (145)	62 Sm 150.35	63 Eu 151.96	64 Gd 157.25	65 Tb 158.92	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.04	71 Lu 174.97
Actinide series	89 Ac (227)	90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)

Increasing electronegativity

Electronegative elements

- Easily take up or share electrons
- Become negatively charged, e.g.

$$Cl + e^{-} \rightarrow Cl^{-}$$

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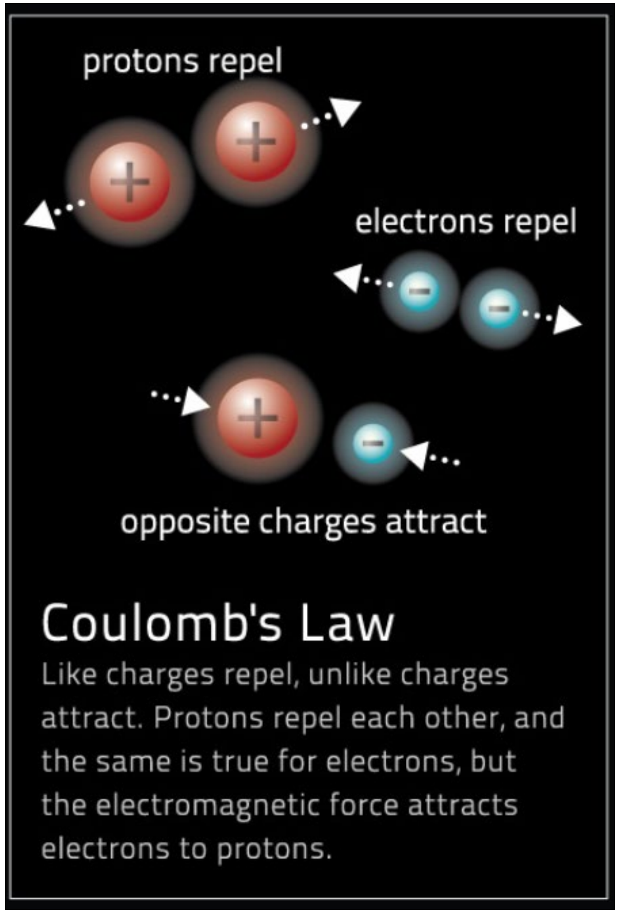
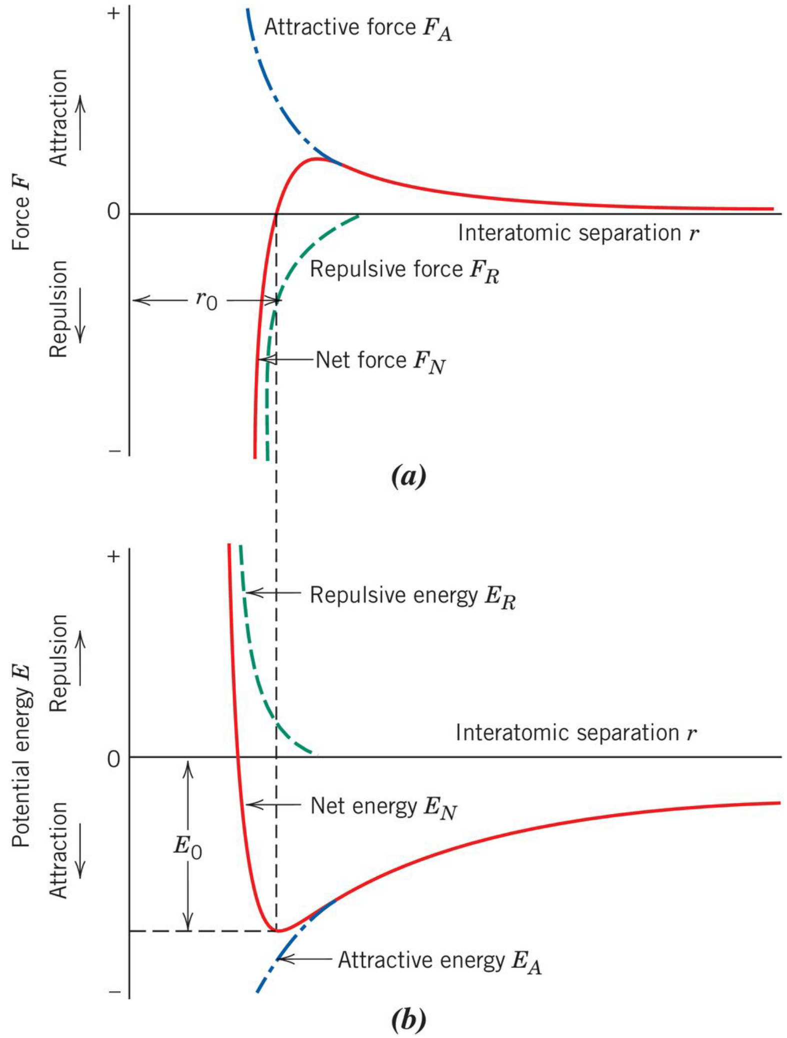
Atomic bonding



Source: https://ecuip.lib.uchicago.edu/multiwavelength-astronomy/astrophysics/05.html



The **net force** acting on two atoms brought very close together is

$$F_A + F_R = F_N$$

When this **force is zero**, the forces are in equilibrium and the interatomic spacing is r_0, **the equilibrium spacing** ($\sim$0.3 nm).

The **net potential energy** between the two atoms can also be determined

$$E_A + E_R = E_N$$

and is at a **minimum at r_0**, with a value of E_0.

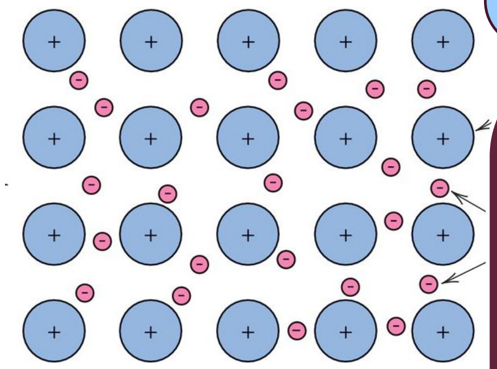
E_0 is the bonding energy of the two atoms and represents the energy required to move the two atoms infinitely apart, i.e. break their bond.

Callister 2.5

Engineering materials: Primary atomic bonds

Metallic bonding

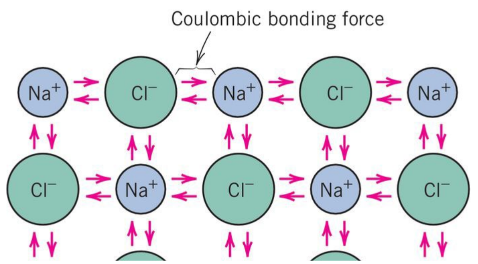
valence electrons are not bound to any particular atom in the solid and are more or less free to drift throughout the entire metal

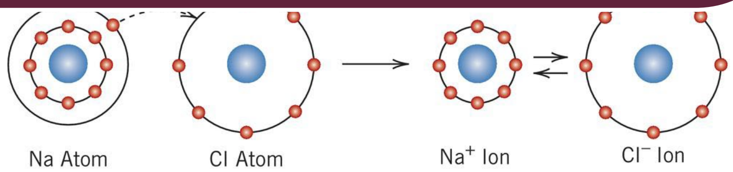


Metals are good conductors of both electricity and heat as a consequence of their free electrons (see Sections 19.5, 19.6, and 20.4). Furthermore, in Section 9.4, we note that at room temperature, most metals and their alloys fail in a ductile manner—that is, fracture occurs after the materials have experienced significant degrees of permanent deformation. This behavior is explained in terms of deformation mechanism (Section 9.2), which is implicitly related to the characteristics of the metallic bond.

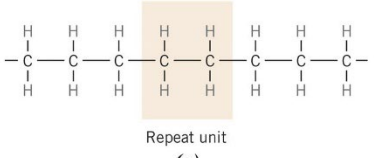
Callister p.37

Ionic bonding

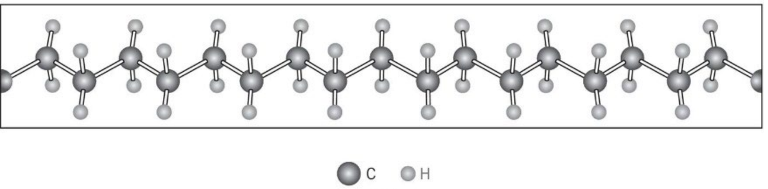




Covalent bonding



(a)



(b)

- Two elements close to each other on periodic table (small electronegativity difference) share valence electrons
- Strong bond

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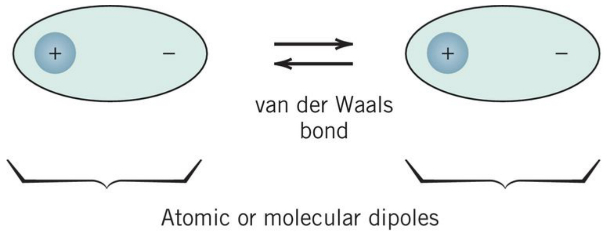
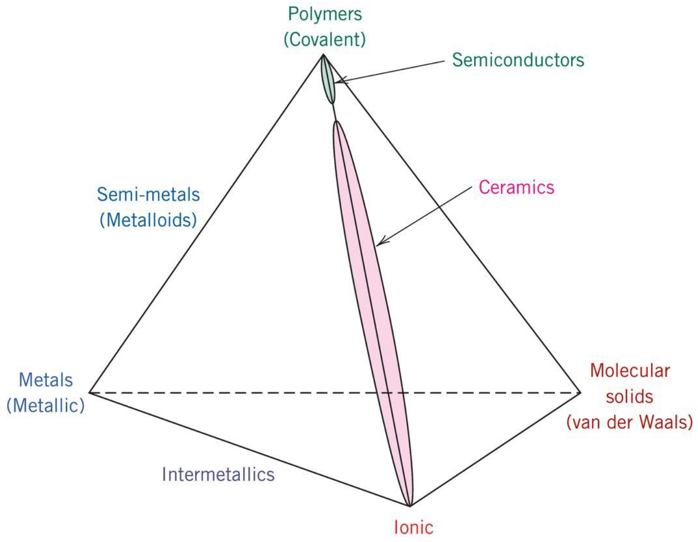
Secondary van der Waals bonding



- Read Chp 2.6 to take note of different types of secondary bonds that form between atomic or molecular dipoles

Mixed bonding



- Read Chp 2.7 to take note that materials can have mixed bonds:
  - Covalent - ionic: most ceramics
  - Covalent – metallic
  - Metallic - ionic

Callister 2.6 – 2.7

An important distinction:

What is the difference between an atom, a molecule, a compound and an ion?

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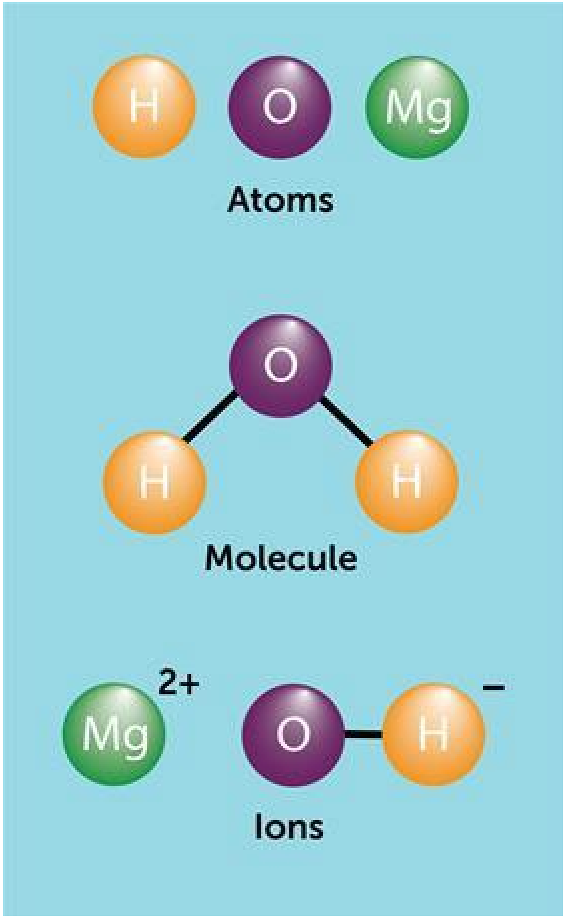

Source: https://edu.rsc.org/cpd/atoms-molecules-and-ions/3010574.article

- Particles can be atoms, molecules or ions.
- Atoms are single neutral particles.
- Molecules are neutral particles made of two or more atoms bonded together.
- Compounds are special types of molecules where two or more DIFFERENT atoms are bonded together.
- An ion is a positively or negatively charged particle.

*When two **atoms** of hydrogen bond, they form a **hydrogen molecule H_2**. When an atom of hydrogen gives up its electron, it forms a **hydrogen ion H^+**. Similarly, when an atom of oxygen takes up two electrons it forms an **oxygen ion O^{2-}**.When 2 atoms of hydrogen form a covalent bond with an oxygen atom, it forms the **water molecule H_20** which is a **compound** of hydrogen and oxygen.*

Thank you | Dankie | Enkosi

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