CHAPTER 2

A little bit of chemistry

Chapter Outline

- **Review of Atomic Structure**

1. Electrons, protons, neutrons
2. Quantum mechanics of atoms (not the scary stuff)
3. Electron states, the periodic Table

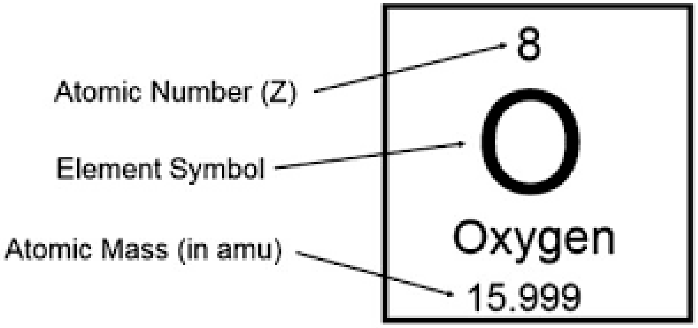
- **Atomic Bonding in Solids**

1. Bonding energies and forces

Atomic structure

Atoms = nucleus (protons and neutrons) + electrons

The atomic mass (A) = mass of protons + mass of neutrons



atomic number (Z) = # protons

The atomic mass (Ar) = is often used to express atomic weight. The atomic mass is a weighted average of all of the isotopes of that element.

A mole is the amount of matter that has a mass in grams equal to the atomic mass in amu of the atoms.
The number of atoms in a mole is called the Avogadro number
Nav = 6.023×10^{23}.

Examples

- Calculate the number of atoms in 1 g of Cu?

Ar (Cu)= 63.54 g/mol

- If there are 3.058×10^{21} atoms present in 1g of gold. Determine the atomic mass of gold.
- Thin gold film (Thickness 50 nm) was sputtered on a smooth Al2O3 substrate. For the total surface area of the gold film (5 cm^2) calculate:

a) Number of gold atoms

b) Moles of gold per unit of surface area

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$N_{av} = 6.023 \times 10^{23}$ atoms/mol

Examples

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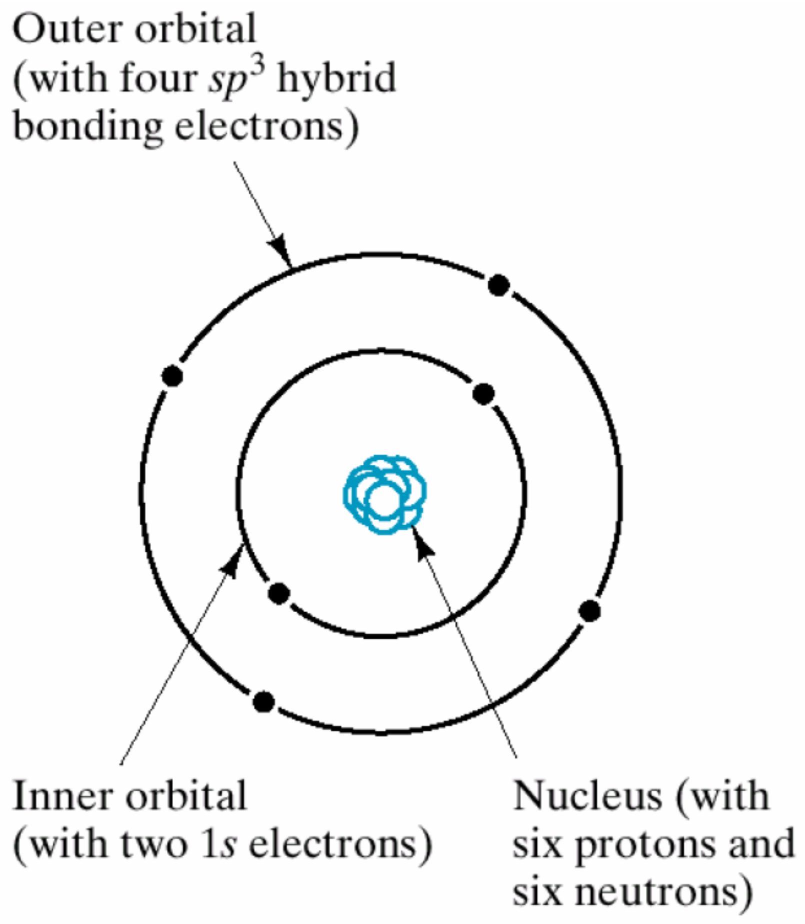
Ar (Au)= 196.97 g/mol
d (thickness)= 5×10^{-6} cm
S (surface area)= 5 cm^2
ρ (density)=19.302 g/cm^3
Nav = 6.023×10^{23} atoms/mol

b) Moles of gold per unit of surface area

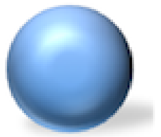
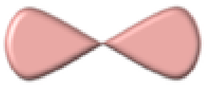
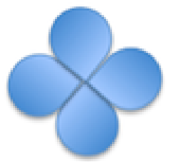
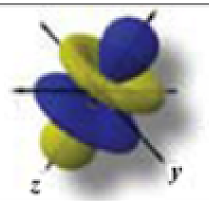
n= 1.476×10^{18} atoms
S (surface area)= 5 cm^2
Nav = 6.023×10^{23} atoms/mol

Electrons in Atoms

- The electrons form a cloud around the nucleus, of radius of 0.05 – 2 nm
- Electrons move not in circular orbits, but in 'fuzzy�much' orbits.
- Electrons occupy discrete energy levels or shells
- Each e- has a particular energy level wit no more than 2 e- with the same energy (Pauli Exclusion Principle)



Electrons in Atoms

Angular Momentum Quantum Number, ℓ	Name of Subshell	Shape	
0	s	Sphere	
1	p	Dumbbell	
2	d	Complex/double dumbbell	
3	f	More complex/ multiple lobes	

- Quantum #'s

n (Principal number)= position of the e^- within the atom (shell) e.g 1, 2, 3, 4.....

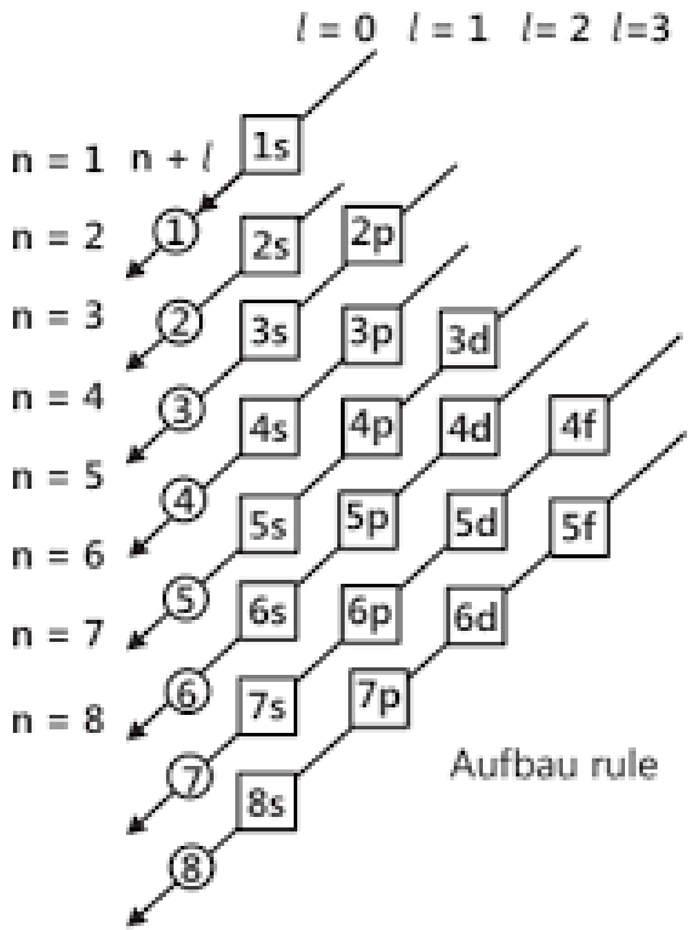
l (Azimuthal number)= position of the e^- within the shell (Subshell) e. g. s, p, d, f

m_l (Magnetic number)= description of the orbital within the subshell

m_s (Spin number)= the direction of the ration of the e^- e.g. +1/2 or -1/2

Electrons in Atoms

- **Aufbau Principle**



Valence electrons Electrons that occupy the outermost filled shell they are responsible for bonding.

Electrons fill quantum levels in order of increasing energy (only n, l make a significant difference).Following Aufbau principal

s=2
p=6
d= 10
f= 14

PERIODIC TABLE OF ELEMENT

2 **He** Helium 4	
	← Proton number ← Symbol ← Name of element ← Relative atomic mass

1 **H** Hydrogen 1																	2 **He** Helium 4
2 **Li** Lithium 3	3 **Be** Beryllium 9											5 **B** Boron 11	6 **C** Carbon 12	7 **N** Nitrogen 14	8 **O** Oxygen 16	9 **F** Fluorine 19	10 **Ne** Neon 20
11 **Na** Sodium 23	12 **Mg** Magnesium 24											13 **Al** Aluminum 27	14 **Si** Silicon 28	15 **P** Phosphorus 31	16 **S** Sulfur 32	17 **Cl** Chlorine 35.5	18 **H** Argon 40
19 **K** Potassium 39	20 **Ca** Calcium 40	21 **Sc** Scandium 45	22 **Ti** Titanium 48	23 **V** Vanadium 51	24 **Cr** Chromium 52	25 **Mn** Manganese 55	26 **Fe** Iron 56	27 **Co** Cobalt 59	28 **Ni** Nickel 59	29 **Cu** Copper 64	30 **Zn** Zinc 65	31 **Ga** Gallium 70	32 **Ge** Germanium 73	33 **As** Arsenic 75	34 **Se** Selenium 79	35 **Br** Bromine 80	36 **Kr** Krypton 84
37 **Rb** Rubidium 86	38 **Sr** Strontium 88	39 **Y** Yttrium 89	40 **Zr** Zirconium 91	41 **Nb** Niobium 93	42 **Nb** Niobium 96	43 **Tc** Technetium 98	44 **Ru** Ruthenium 101	45 **Rh** Rhodium 103	46 **Pd** Palladium 106	47 **Ag** Silver 108	48 **Cd** Cadmium 112	48 **In** Indium 115	50 **Sn** Tin 119	51 **Sb** Antimony 122	52 **Te** Tellurium 128	53 **I** Iodine 127	54 **Xe** Xenon 131
55 **Cs** Cesium 133	56 **Ba** Barium 137	57 **La** Lanthanum 139	72 **Hf** Hafnium 179	73 **Ta** Tantalum 181	74 **W** Tungsten 184	75 **Re** Rhenium 186	76 **Os** Osmium 190	77 **Ir** Iridium 192	78 **Pt** Platinum 195	79 **Au** Gold 197	80 **Hg** Mercury 201	81 **Ti** Thallium 204	82 **Pb** Lead 207	83 **Bi** Bismuth 209	84 **Po** Polonium 210	85 **At** Astatine 210	86 **Rn** Radon 222
87 **Fr** Francium 223	88 **Ra** Radium 226	89 **Ac** Actinium 227	104 **Unq** Unnilquadium 257	105 **Unp** Unnilpentium 260	106 **Unh** Unnilhexium 263	107 **Uns** Unnilseptium 262	108 **Uno** Unniloctium 265	109 **Une** Unnilennium 266									

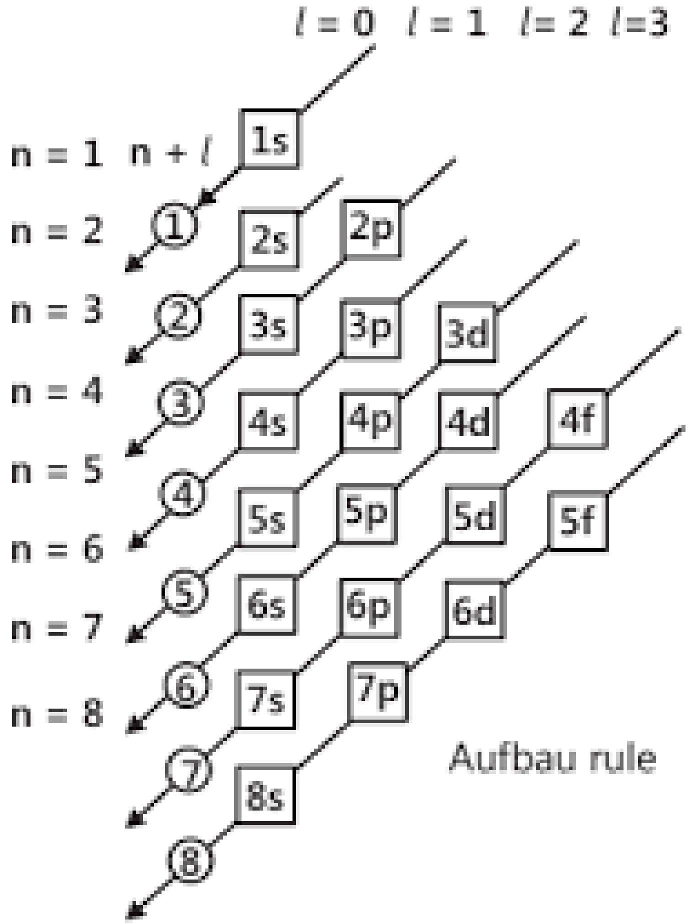
58 **Ce** Cerium 140	59 **Pr** Praseodymium 141	60 **Nd** Neodymin 144	61 **Pm** Promethium 147	62 **Sm** Samarium 150	63 **Eu** Europium 152	64 **Gd** Gadolinium 157	65 **Tb** Terbium 159	66 **Dy** Dysprosium 136	67 **Ho** Holmium 165	68 **Er** Erbium 167	69 **Tm** Thulium 169	70 **Yb** Yuterbium 173	71 **Lu** Lutertium 175
90 **Th** Thorium 232	91 **Pa** Proactinum 231	92 **U** Uranium 238	93 **Np** Neptunium 237	94 **Pu** Plutonium 244	95 **Am** Americium 243	96 **Cm** Curium 247	97 **Bk** Berkerium 247	98 **Cf** Californium 249	99 **Es** Einsteinium 254	100 **Fm** Fermium 253	101 **Md** Mendelevium 256	102 **No** Nobelium 254	103 **Lr** Lawrensium 257

Examples

- Find the electronic distribution Ar and Fe
- Find the valence electrons in Aluminum and Germanium

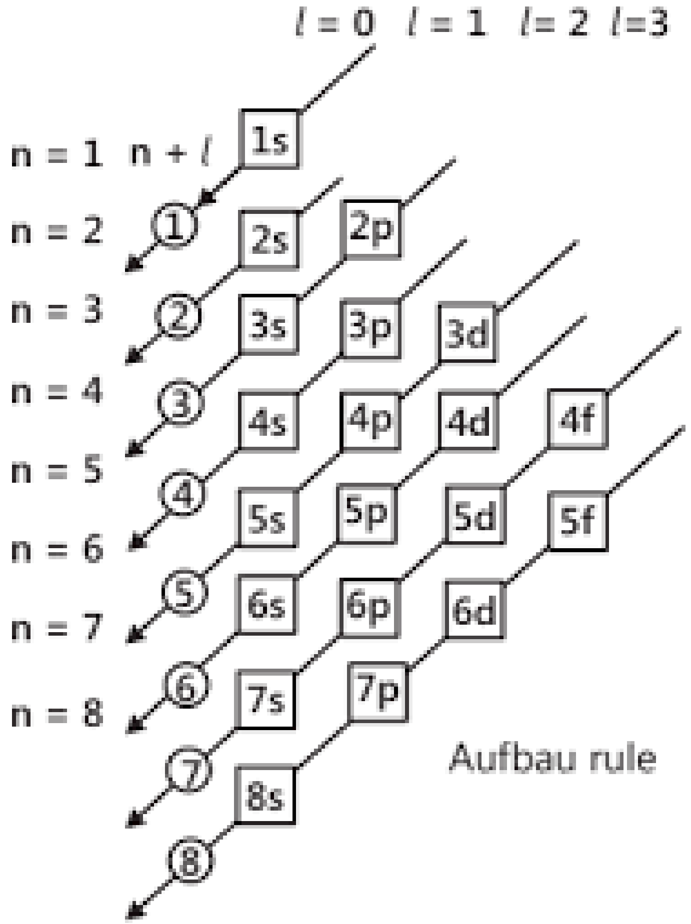
Find the electronic distribution Ar and Fe

Z (Ar)= 18
Z (Fe)= 26



Find the valence electrons in Aluminum and Germanium

Z (Al)= 13
Z (Ge)= 32

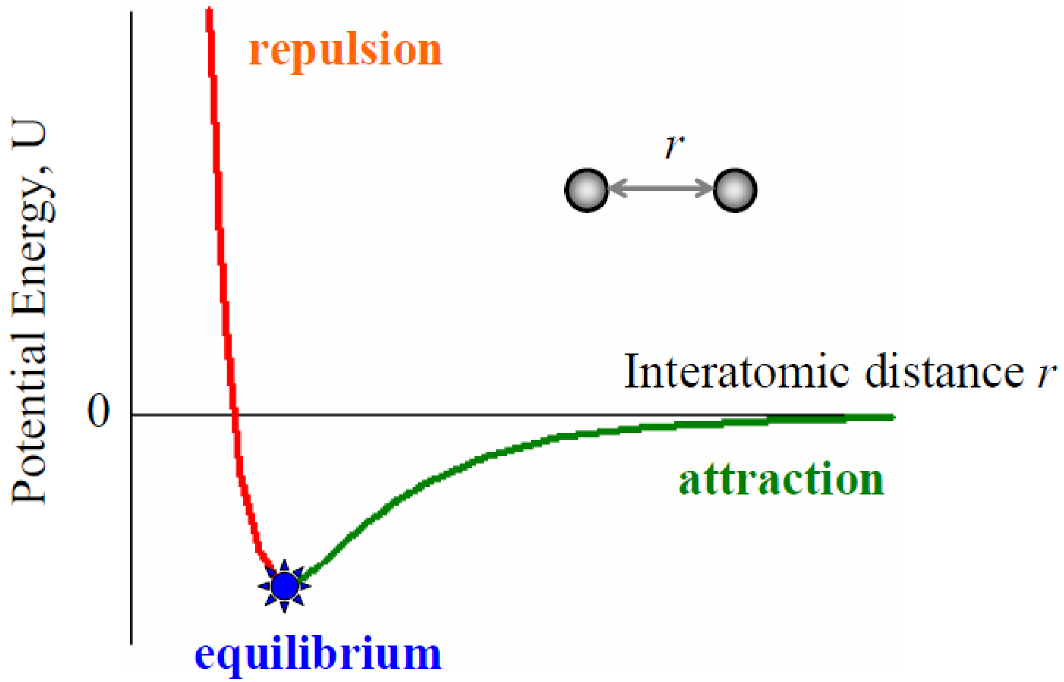


Atomic bonding

Electronegativity - a measure of how willing atoms are to accept electrons

The repulsion between atoms, the electronic clouds surrounding the atoms starts to overlap.

The origin of the attractive part depends on the particular type of bonding.

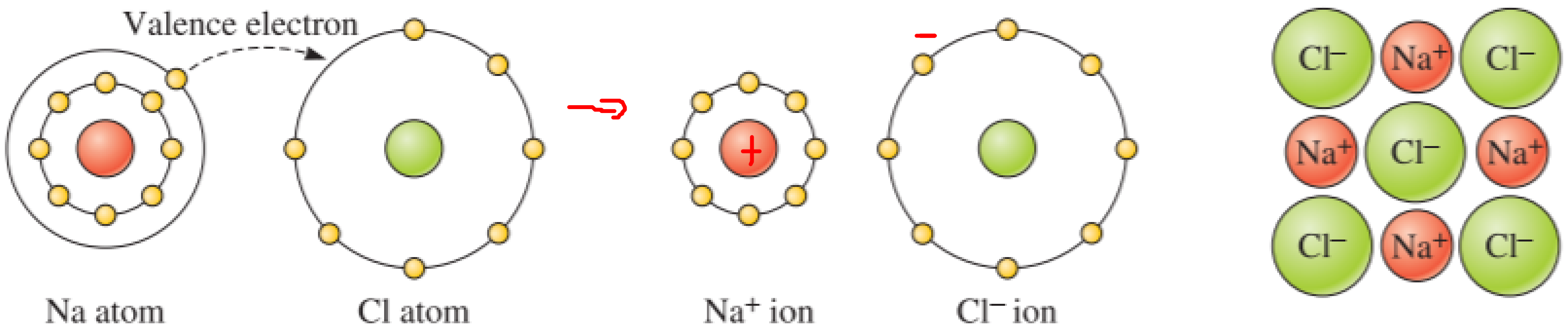


Types on Bonding

- Ionic: Strong Coulomb interaction among negative atoms (have an extra electron each) and positive atoms (lost an electron). Example - Na^+Cl^-
- Covalent: electrons are shared between the molecules, to saturate the valency. Example - H_2
- Metallic: the atoms are ionized, loosing some electrons from the valence band. Those electrons form an electron sea, which binds the charged nuclei in place.
- Van der Waals: Secondary , weak bonding

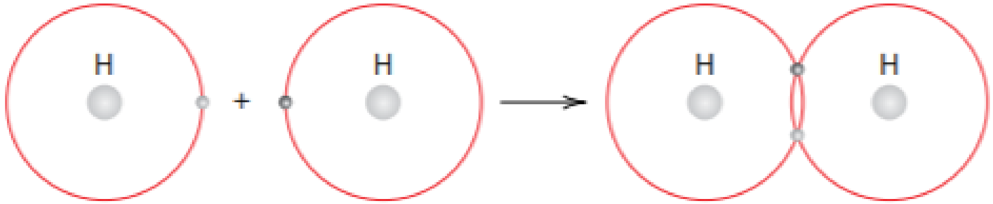
Ionic Bond

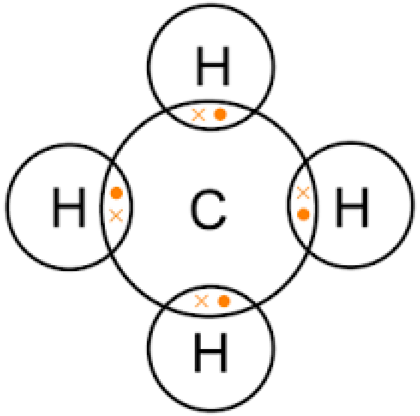
- It is always found in compounds composed of both metallic and nonmetallic elements.
- One atom may donate its valence electrons to a different atom, filling the outer energy shell of the second atom.
- Both atoms now have an electrical charge and behave as ions. The atom that contributes the electrons is left with a net positive charge and is called a **cation**, while the atom that accepts the electrons acquires a net negative charge and is called an **anion**.
- The oppositely charged ions are then attracted to one another and produce the ionic bond.



Covalent bond

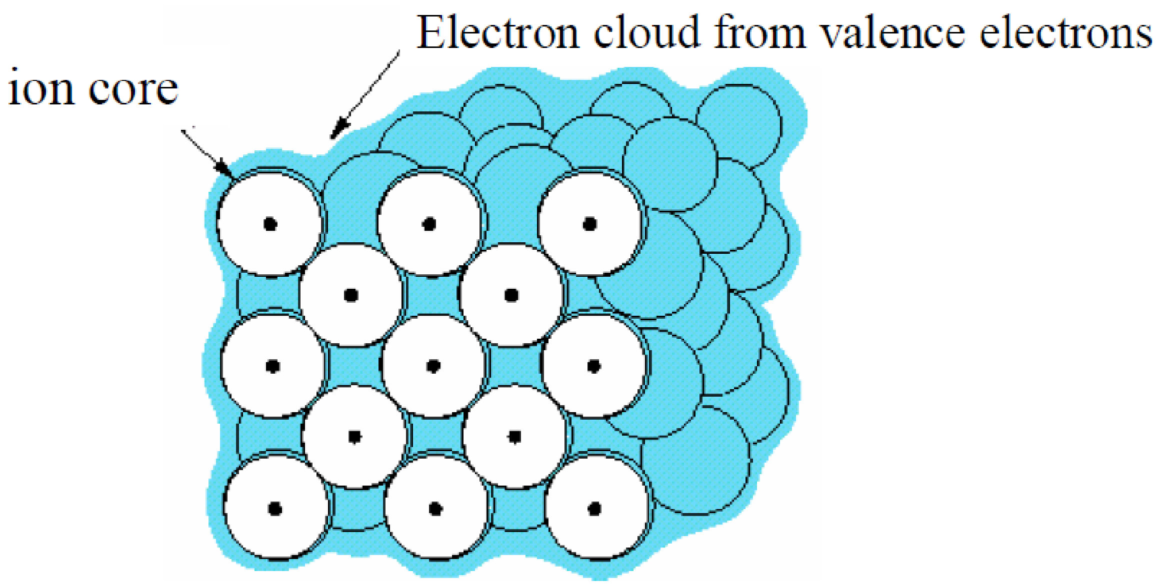
- Found in materials whose atoms have small differences in electronegativity (near one another in the periodic table).
- Formed by sharing of valence electrons among two or more atoms.
- The ions repel each other but are attracted to the electrons that spend most of the time in between the ions. Can be described by orbital overlap





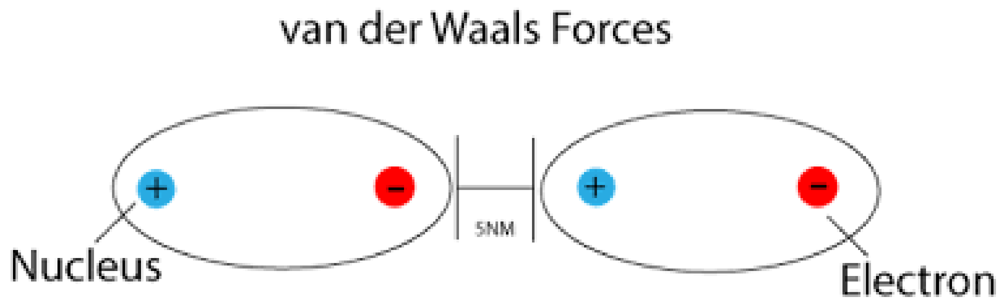
Metallic Bond

- The valence e- are not bound to any particular atom and are free to drift throughout the entire metal.
- They may be thought of as belonging to the metal as a whole ("electron cloud or sea").
- The remaining nonvalence e- and atomic nuclei form what are called ion cores, it has net positive charge equal in magnitude to the total valence e- charge



Van der Waals

- Secondary bonds are weak in comparison to primary bonds.
- They are found in most materials, but their effects are often overshadowed by the strength of the primary bonding.
- Formed when an uneven charge distribution occurs, creating what is known as a dipole (the total charge is zero, but there is slightly more positive or negative charge on one end of the atom than on the other).



Examples of bonding in Materials:

- Metals: Metallic
- Ceramics: Ionic / Covalent
- Polymers: Covalent and Secondary
- Semiconductors: Covalent or Covalent / Ionic