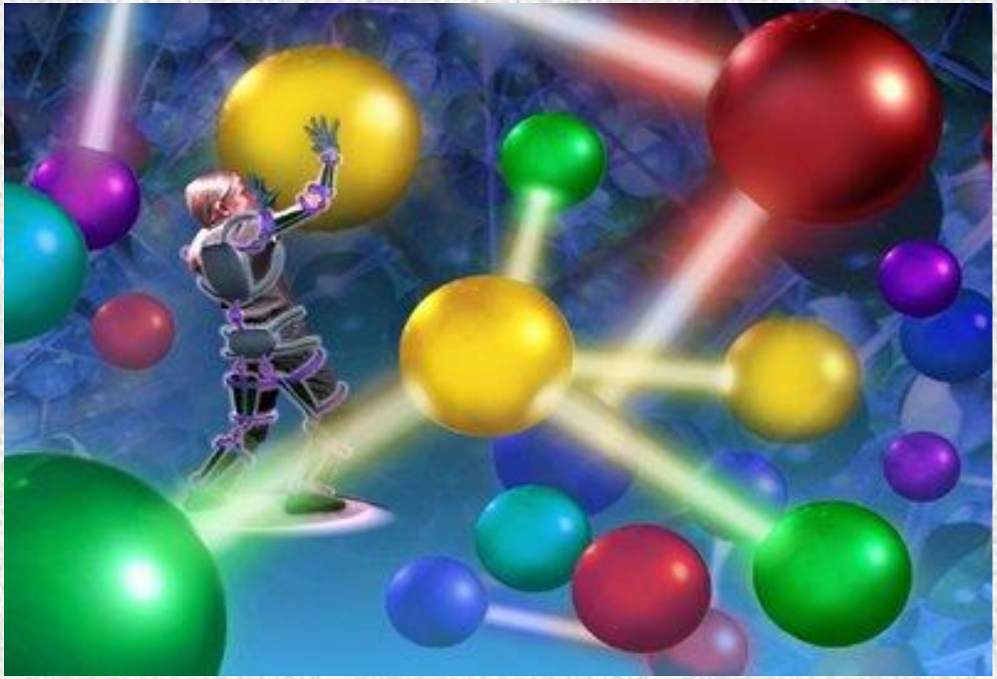
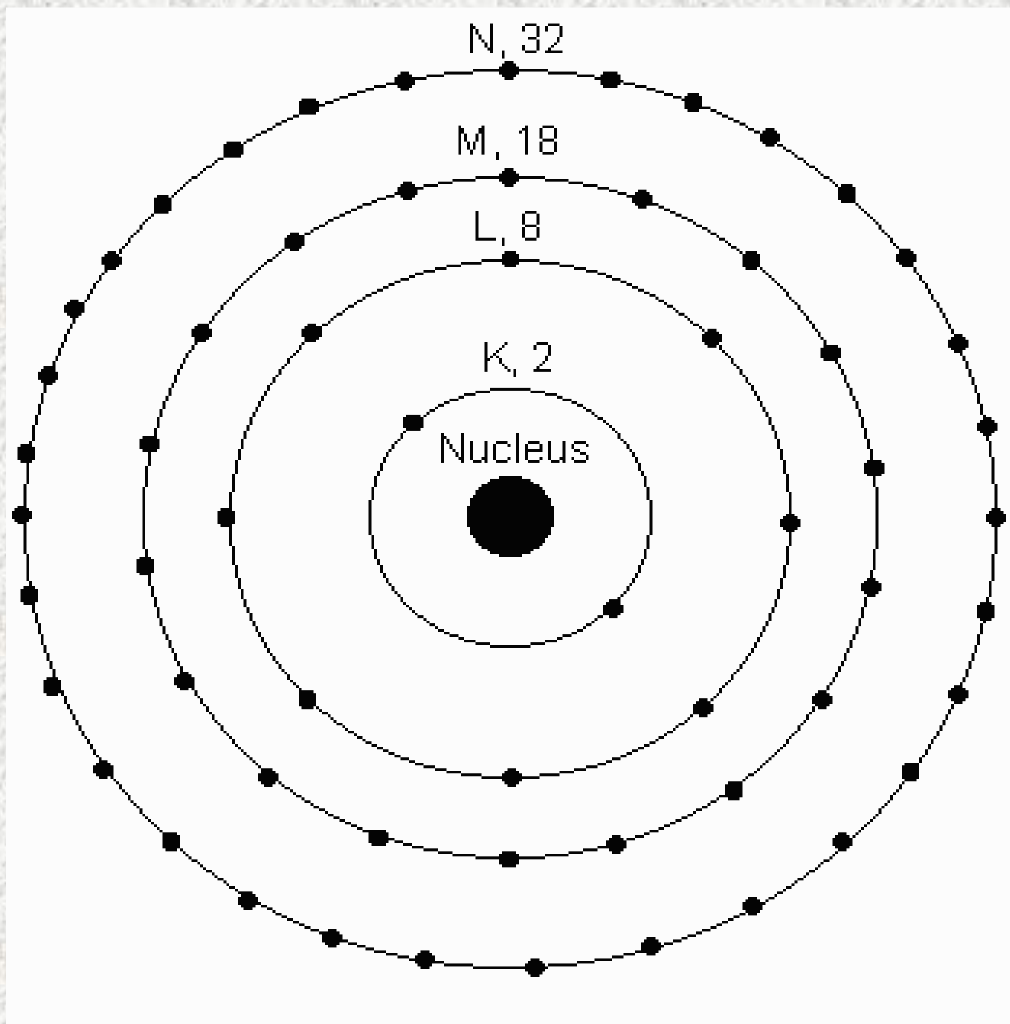
Atomic bonding



Primer Materials For Science Teaching

Spring 2020

Atom Structure

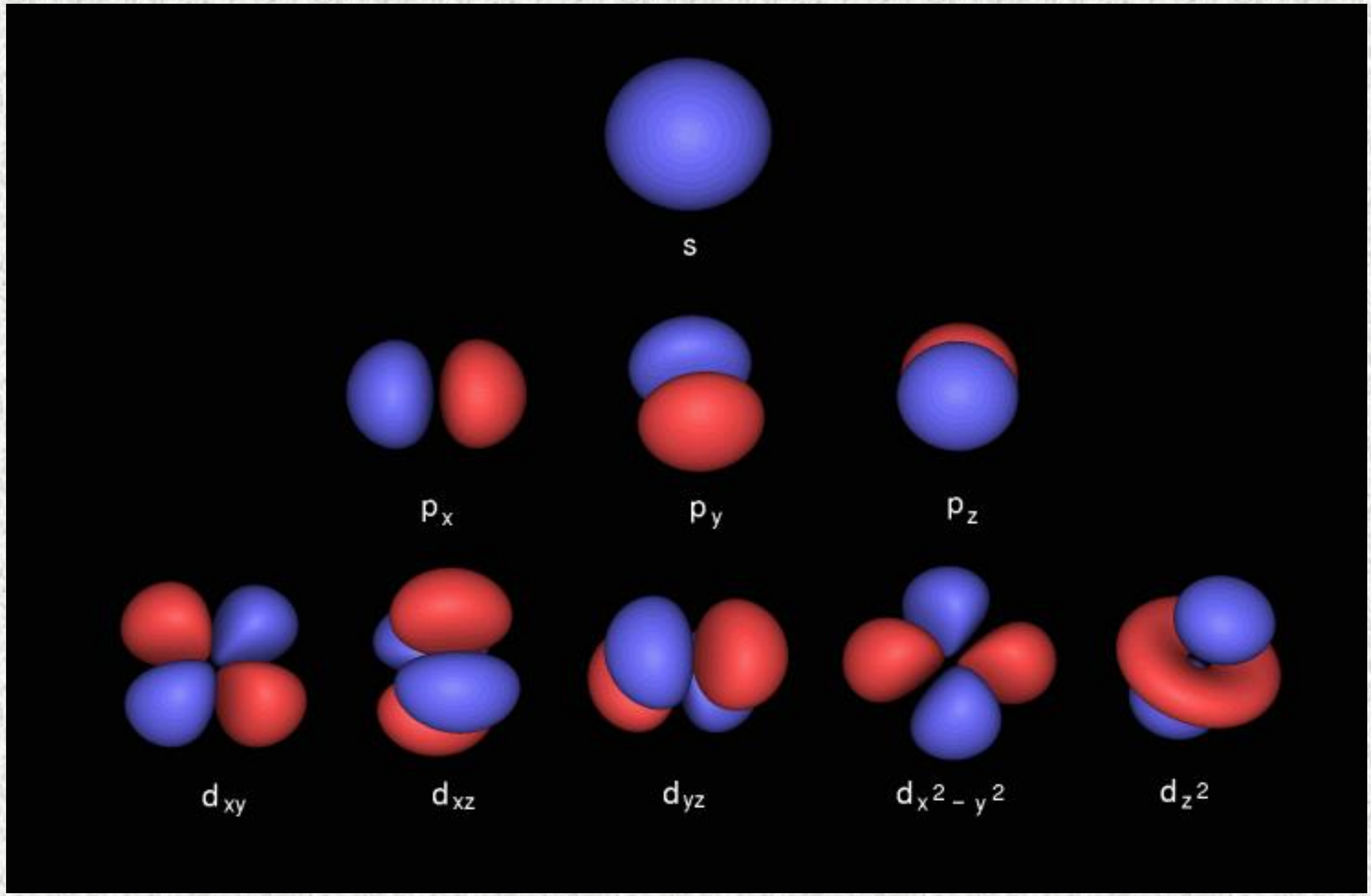


Quantum numbers

The energy level to which each electron belongs is determined by four quantum numbers

- n – this principle quantum number assigned integral values 1, 2, 3, 4, 5 , … that refer to the quantum shell to which the electron belongs. Quantum shells are also assigned a letter. n=1 is K, n=2 is L, n=3 is M, on so on
- l - is the azimuthal quantum number which determines the angular momentum of the electron. l= 0,1,2,…n-1. the azimuthal quantum numbers are designated by lower case letters. s for l=0, p for l=1, d for l=2, f for l=3, etc
- There are another two quantum numbers: m_l=-l…-1,0,1…l; m_s=1/2, -1/2 (for electron)

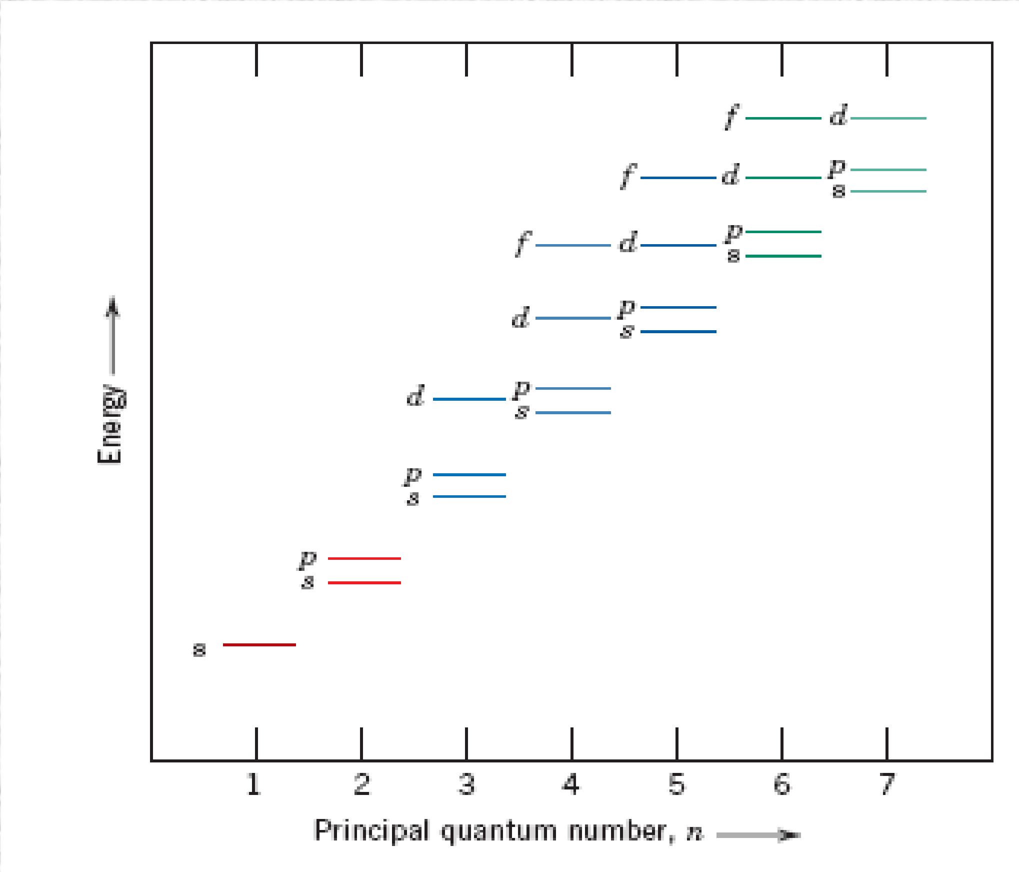
Atomic Orbital



Electronic population in subshells

Pauli exclusion principle: **two or more electrons with the same quantum numbers cannot occupy the same energy level in the atom**

Relative energies of the electrons for the various shells and sub-shells



Valance

- **The valance relates to the ability of an atom to enter into chemical combination with other elements**
- **Valance is often determined by the number of electrons in the outmost combined *sp* level**
- Mg: $1s^2 2s^2 2p^6 3s^2$ valance = 2
- Al: $1s^2 2s^2 2p^6 3s^2 3p^1$ valance = 3
- P : $1s^2 2s^2 2p^6 3s^2 3p^3$ valance = 5
- Ge: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^2$ valance = 4
- **Valance may depends of the nature of the chemical reaction.**

Electronegativity

- If an atom has a valance of zero, the element is inert, for example:
    - Ar: $1s^2 2s^2 2p^6 3s^2 3p^6$ Valance - 0
- Other atoms prefer to behave as if their outer *sp* levels are either completely full or completely empty.
- Electonegativity describes the tendency of an atom to gain an electron

Periodic table sorted by Electronegativity

The electronegativity values for the elements.

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII	VIII	VIII	IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
1 H 2.1																	2 He –
3 Li 1.0	4 Be 1.5											5 B 2.0	6 C 2.5	7 N 3.0	8 O 3.5	9 F 4.0	10 Ne –
11 Na 0.9	12 Mg 1.2											13 Al 1.5	14 Si 1.8	15 P 2.1	16 S 2.5	17 Cl 3.0	18 Ar –
19 K 0.8	20 Ca 1.0	21 Sc 1.3	22 Ti 1.5	23 V 1.6	24 Cr 1.6	25 Mn 1.5	26 Fe 1.8	27 Co 1.8	28 Ni 1.8	29 Cu 1.9	30 Zn 1.6	31 Ga 1.6	32 Ge 1.8	33 As 2.0	34 Se 2.4	35 Br 2.8	36 Kr –
37 Rb 0.8	38 Sr 1.0	39 Y 1.2	40 Zr 1.4	41 Nb 1.6	42 Mo 1.8	43 Tc 1.9	44 Ru 2.2	45 Rh 2.2	46 Pd 2.2	47 Ag 1.9	48 Cd 1.7	49 In 1.7	50 Sn 1.8	51 Sb 1.9	52 Te 2.1	53 I 2.5	54 Xe –
55 Cs 0.7	56 Ba 0.9	57–71 La–Lu 1.1–1.2	72 Hf 1.3	73 Ta 1.5	74 W 1.7	75 Re 1.9	76 Os 2.2	77 Ir 2.2	78 Pt 2.2	79 Au 2.4	80 Hg 1.9	81 Tl 1.8	82 Pb 1.8	83 Bi 1.9	84 Po 2.0	85 At 2.2	86 Rn –
87 Fr 0.7	88 Ra 0.9	89–102 Ac–No 1.1–1.7															

Example 1.1

- Using the electronic structure, compare the electronegativities of calcium and bromine

- The electronic structures are:
  - Ca : $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$
  - Br : $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^5$

  Calcium has two electrons in its outer *4s* orbital and bromine has seven in its *4s4p* orbital. Thus calcium, with an electronegativity of 1.0, tends to give up electrons and is strongly electropositive, but bromine with an electronegativity of 2.96, tends to accept electrons and is strongly electronegative.

Bonds in solid

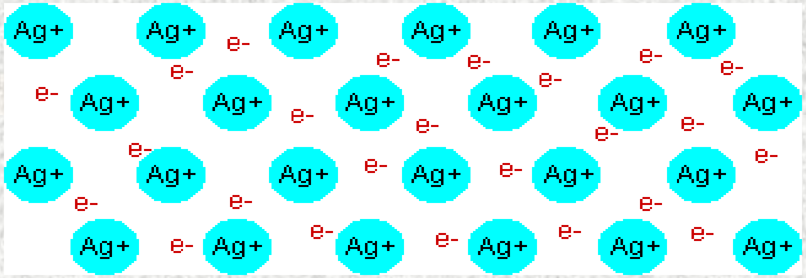
Four important mechanisms by which atoms are bonded in solid

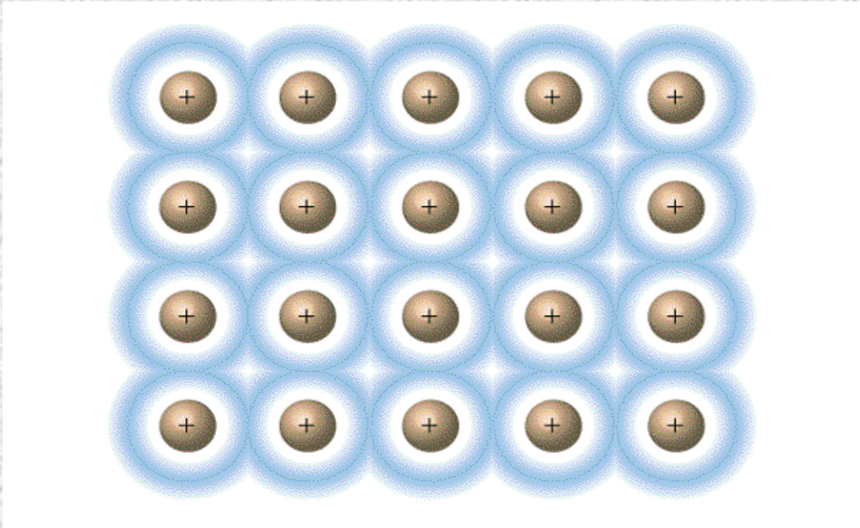
Bond	Binding Energy (kJ per mol)
The metallic bond	625-1550
The covalent bond	520-1250
The ionic bond	100-800
Van der Waals bonding	<40

- Mixed bonding

Metallic Bond

- Each atom gives up its valance electrons and becomes slightly positively charged.
- The negatively charged electrons hold the metal atoms together.
- The electrons are free to move leading to good thermal and electrical conductivity.





Example 1.2

- Calculate the number of electrons capable of conducting an electrical charge in ten cubic centimeter of silver.

Ag: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^1$

silver has only one valance electron hence each atom gives one electron for electric conduction.

From literature we find that: $\rho := 10.49 \frac{gm}{cm^3}$ $\quad Mw := 107.868 \frac{gm}{mol}$ $\quad Av := 6.022 \cdot 10^{23} \frac{1}{mol}$ $\quad V := 10cm^3$

The mass of 10[cm³] of silver is: $M := V \cdot \rho$ $\quad M = 0.105\,kg$

The number of atoms is: $No\_atoms := M \cdot \frac{Av}{Mw}$ $\quad No\_atoms = 5.856 \times 10^{23}$

And there is 1 valance electron/atom,

Number valance electrons = $5.856 \cdot 10^{23}$ in 10 cm^3 of silver

Covalent Bond

The atoms shares the electrons

Carbon –6 electrons

2 electrons in 1s shell (close shell)

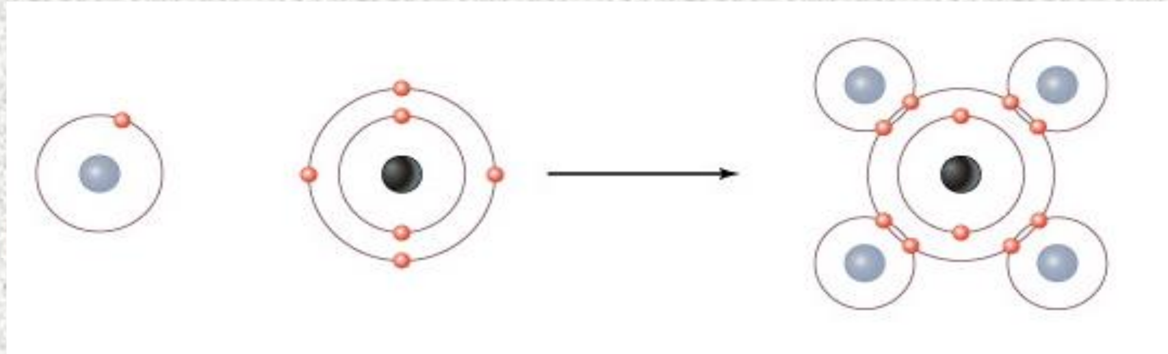
4 electrons in 2s2p shell (lack of four e')

Hydrogen –1 electron in 1s shell (open shell)

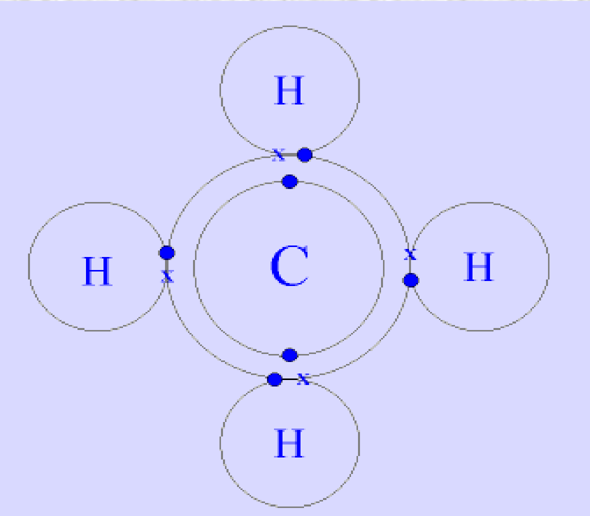
Properties

- Very strong
- Poor electrical conduction

N_2 ,H_2 , O_2, SiO_2, $MgCl_2$



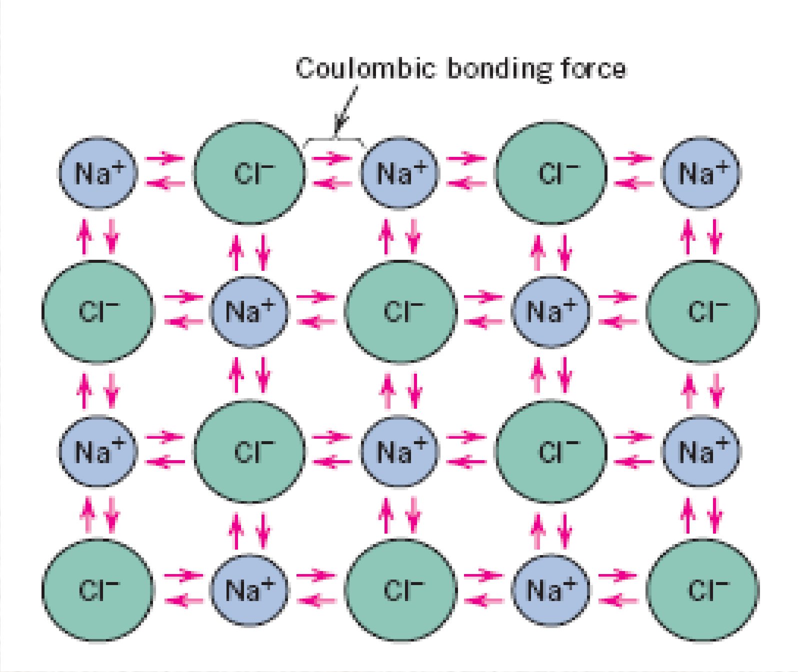
Methane (CH_4) molecule



Ionic bond

- One donate its valance electrons to a different atoms, filling his outer shell
- Electrostatic attraction due to Columb’s law:

$$F = k_e \frac{q_1 q_2}{r^2}$$



Example 1.3

- Describe the ionic bonding between magnesium and chlorine

The electronic structure and valences are:

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

Cl: $1s^2 2s^2 2p^6 3s^2 3p^5$

Mg has two electrons in its open shell which he'll be more than gladly to give them away (and become Mg^{+2} ion) to chlorine who needs only 1 electron in order to close its outer open shell. After the donation one might get chlorine ion Cl^- . The two ions will attached due to columb 's law and the $MgCl_2$ compound will form

Mixed bonds

- In most materials, bonding between atoms is a mixture of two or more types.
- Metals may have combination of metallic and covalent bonding
- Ceramics and semiconductors have mixture of covalent and ionic bonding
- The fraction of bonding that is covalent can be estimated form the equation:

$$\text{Fraction covalent} = \text{Exp}(-0.25 \cdot \Delta E^2)$$

ΔE – difference in electronegativity

Example 1.4

- What is the fraction of the covalent bonding in silica (SiO_2)

First lets estimate the electronegativity of silicon and oxygen:
Si – 1.9
O – 3.44

ΔE=3.44-1.9=1.54

The fraction is: $Exp(-0.25*1.54^2)=0.553$

Pure ionic Vs. Pure covalent

There is a continues range of crystals between the ionic and the covalent limits

Table 8 Fractional ionic character of bonds in binary crystals

Crystal	Fractional ionic character	Crystal	Fractional ionic character
Si	0.00		
SiC	0.18	GaAs	0.31
Ge	0.00	GaSb	0.26
ZnO	0.62	AgCl	0.86
ZnS	0.62	AgBr	0.85
ZnSe	0.63	AgI	0.77
ZnTe	0.61	MgO	0.84
CdO	0.79	MgS	0.79
CdS	0.69	MgSe	0.79
CdSe	0.70		
CdTe	0.67	LiF	0.92
		NaCl	0.94
InP	0.42	RbF	0.96
InAs	0.36		
InSb	0.32		

After J. C. Phillips, *Bonds and bands in semiconductors*.

Van Der Waals bonding

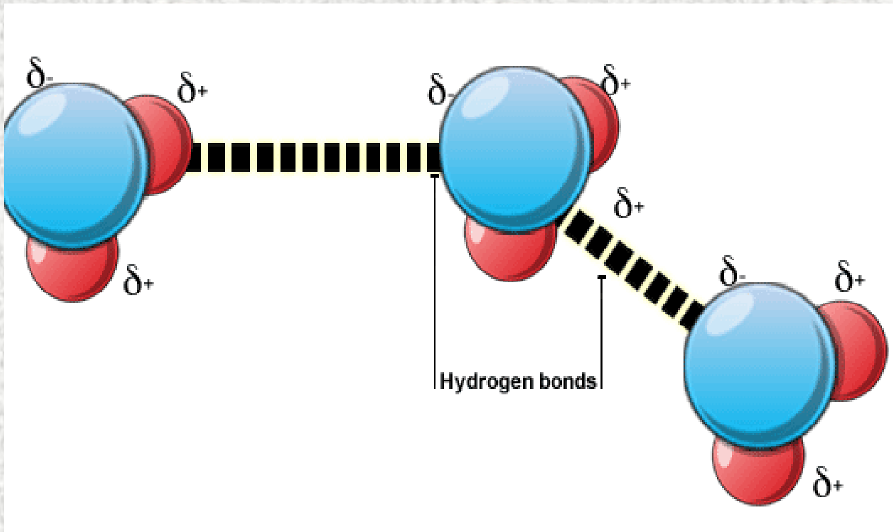
Intermolecular forces which caused by correlations in the fluctuating polarizations of nearby particles

In general, an intermolecular potential has a repulsive component ($E_{rep}=B/r^n$) and an attractive component ($E_{att}=-A/r$), which, in turn, consists of three distinct contributions:

1. The electrostatic interactions between permanent dipoles
2. Induction, which is the interaction between a permanent multi-dipoles on one molecule with an induced multi-dipole on another.
3. Attraction experienced by non-polar atoms, but it is operative between **any pair of molecules**.

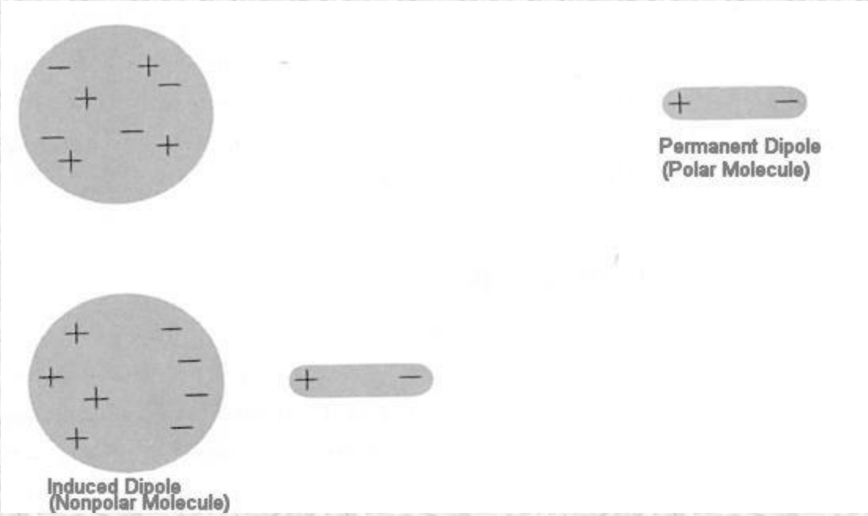
- Weak and short-range interaction

Examples of Van der waals forces



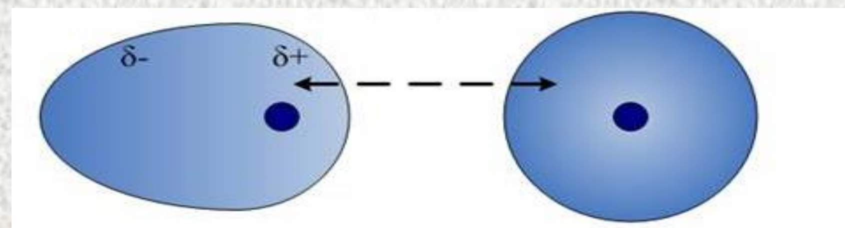
Dipole – dipole interaction (includes hydrogen bonds!)

Dipole – induce dipole interaction

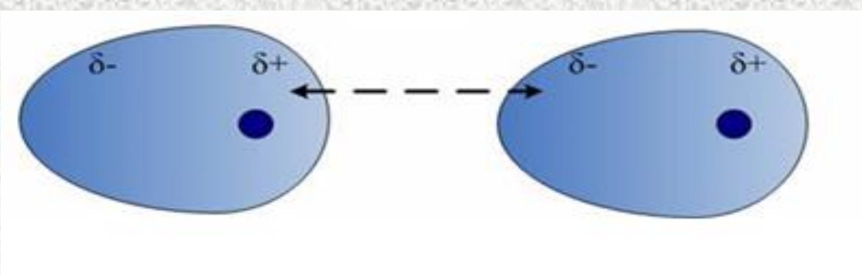


Interaction between symmetric molecules

In general, atoms of an ideal gas should not be attracted nor repelled by on another



Atoms may experience instantaneous dipole moment. Partial charge on one atom cause a neighbouring atom to distort due to the electrostatic attractions/repulsions of their electron cloud

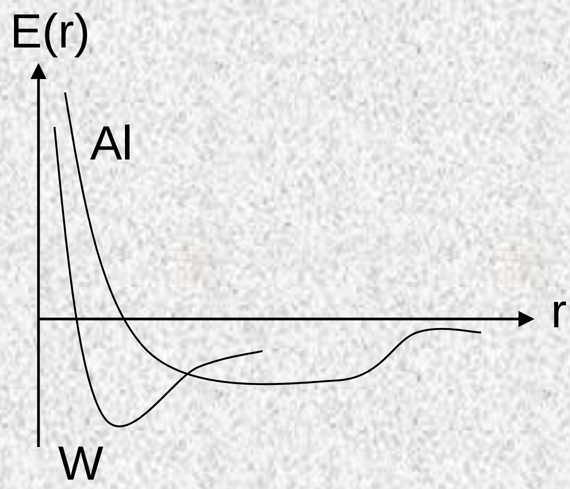


Attraction forces exists between the two induced dipole atoms

Example 1.5

Using the graphs of the interatom potential of tungsten (W) and aluminium (Al), determine:

1. Which of the metals has the lower melting point? Al
2. Which of the metals has the lower heat expansion coefficient? W



Summary of atomic bonding