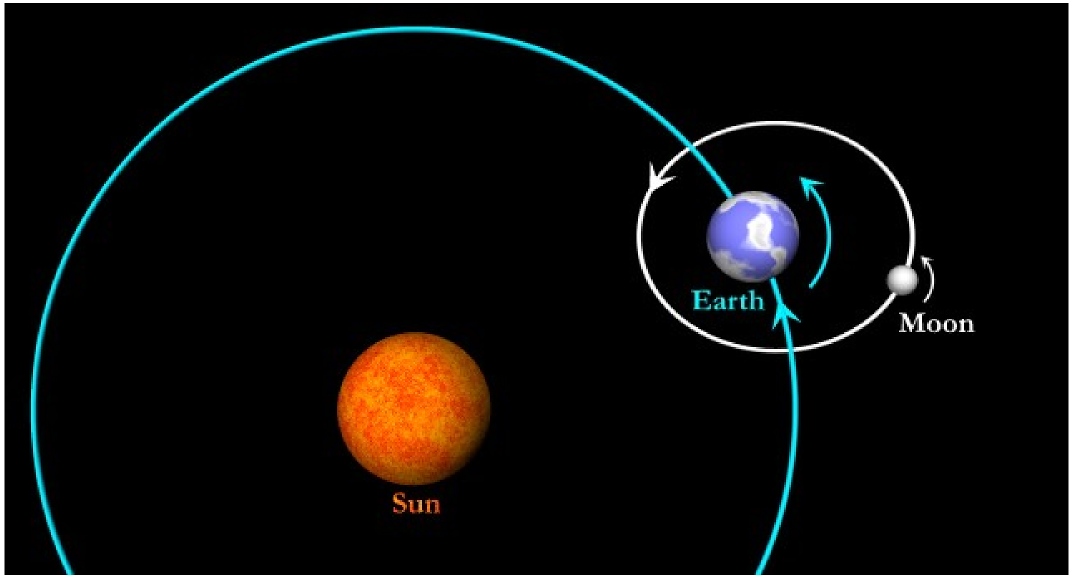
INTRA- & INTER-MOLECULAR BONDS (FORCES)

Serkan GÜRGÜL, Assist. Prof.

Department of Biophysics, Faculty of Medicine, Gaziantep University

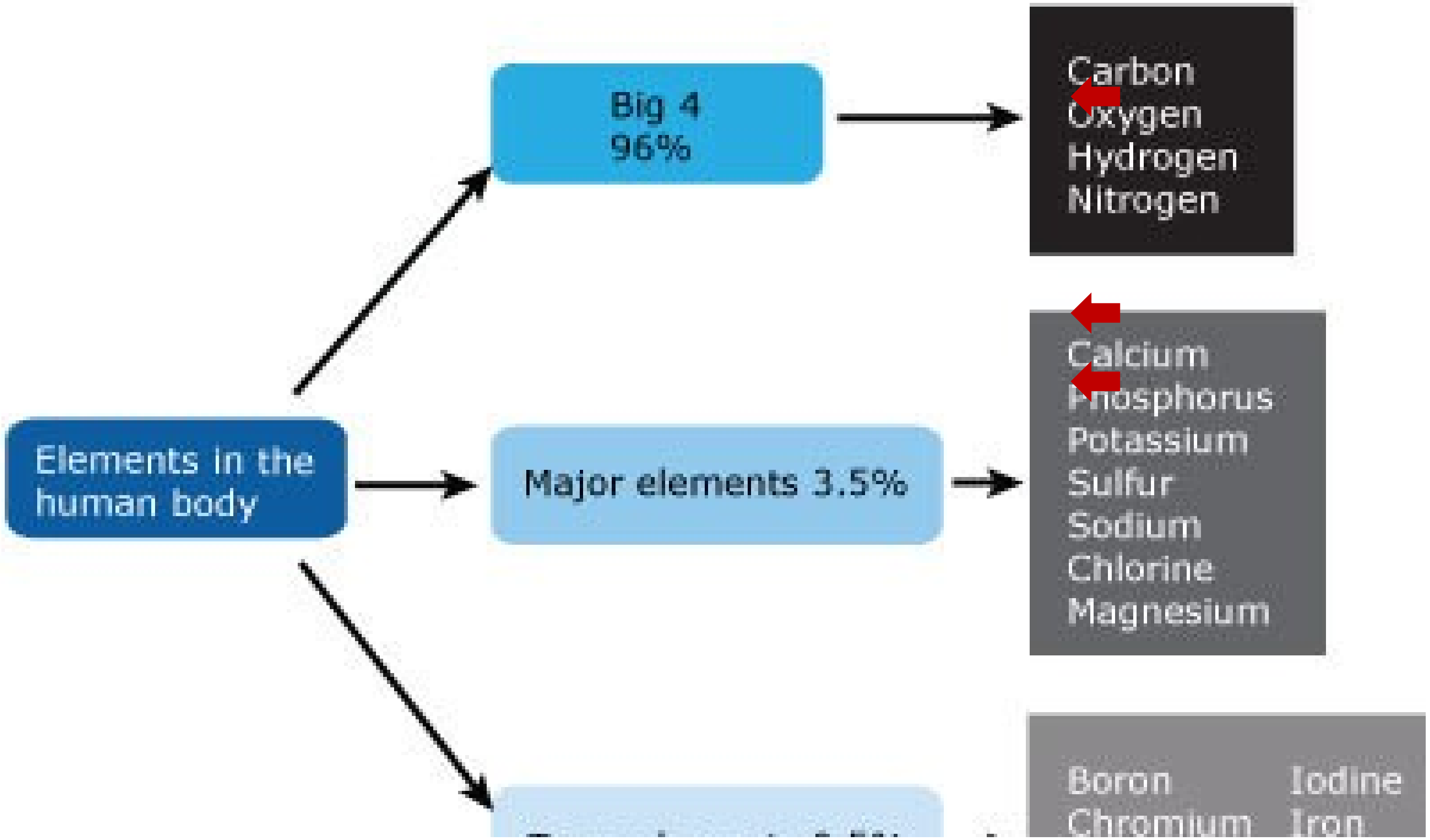
Attractive & Repulsive Forces

- **Some clues** associated with **understanding the microscopic system are hidden behind the macroscopic world**.
- **Eg... Interaction between the Sun and the Earth.**

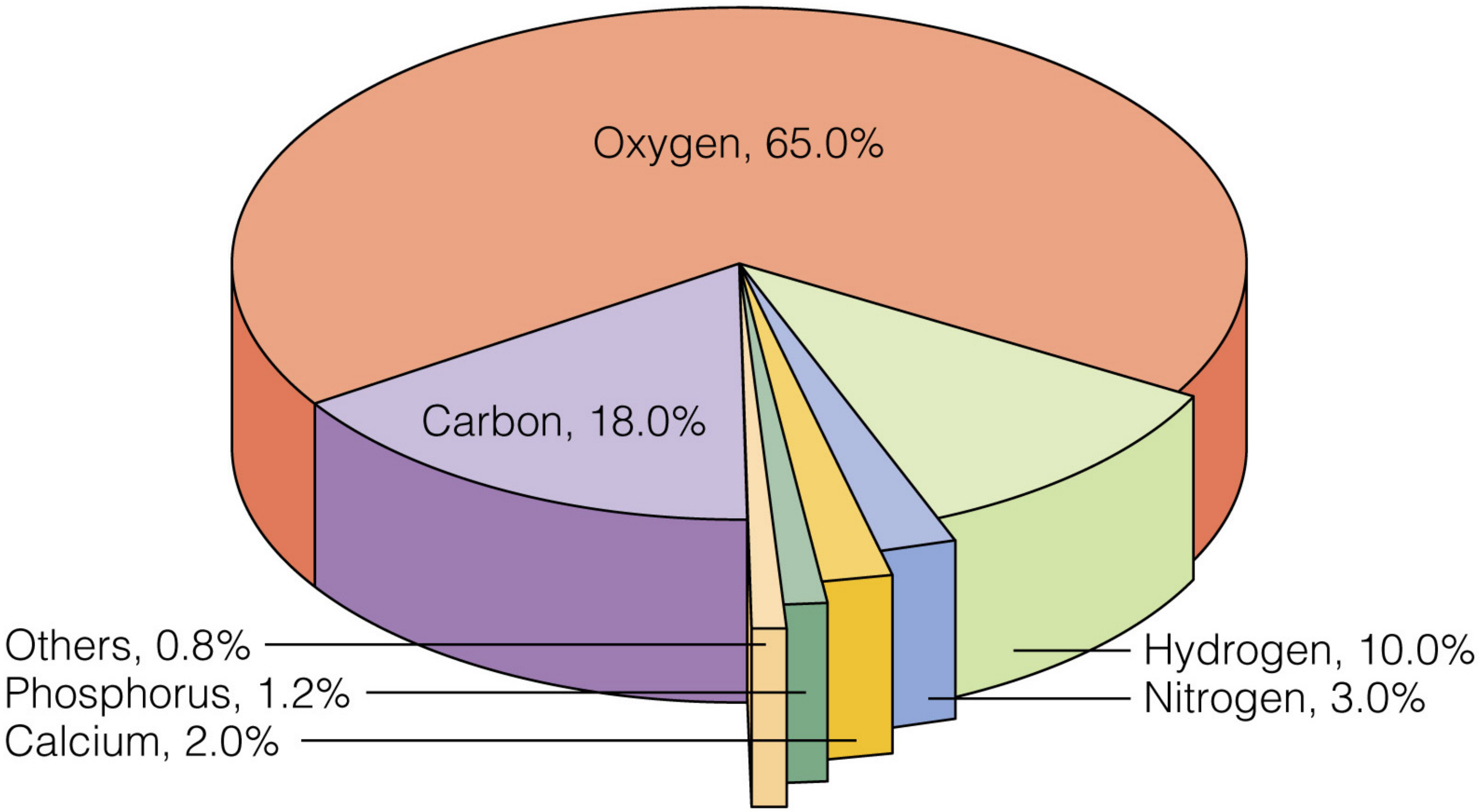


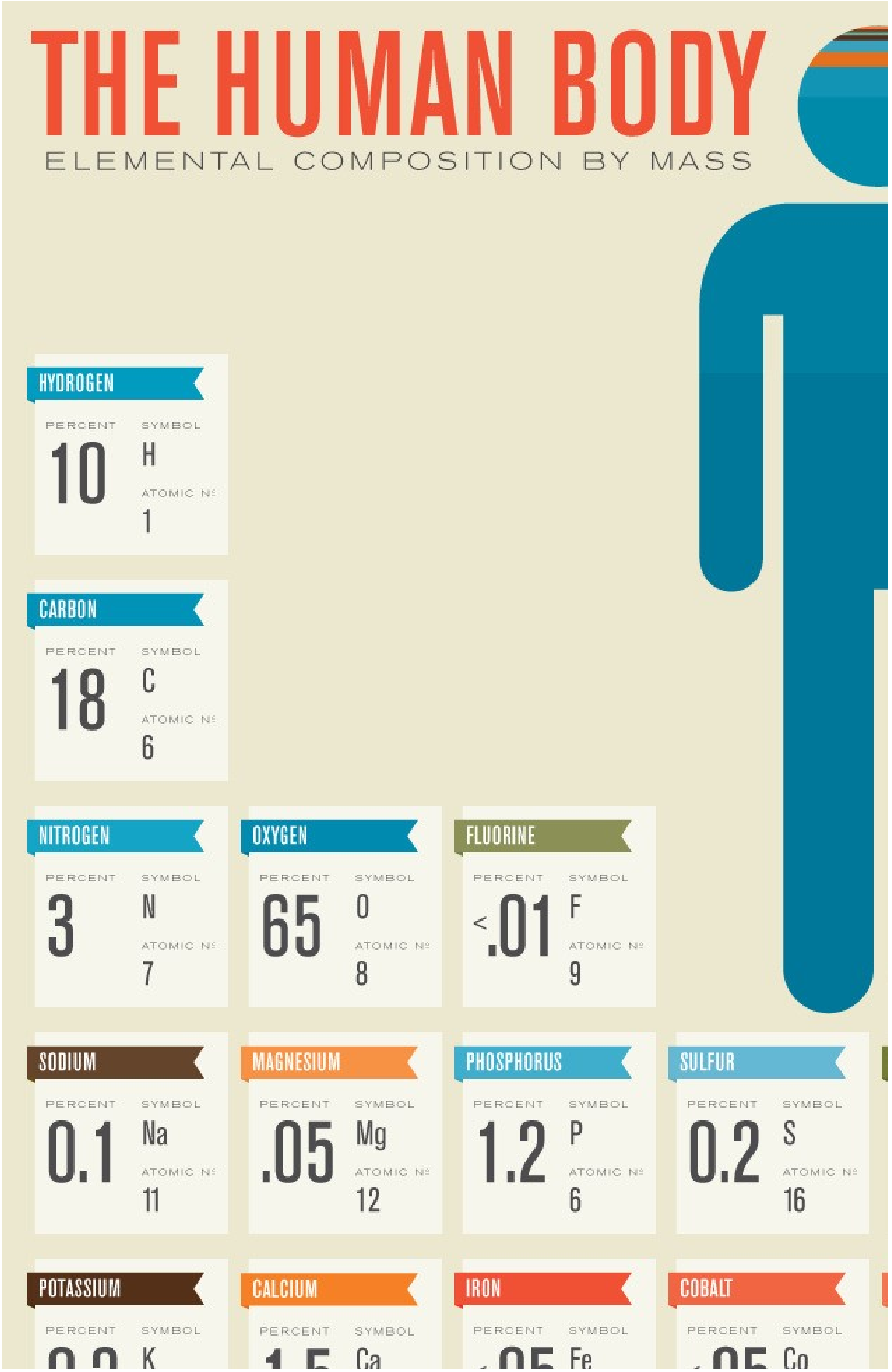
- **The balance of the attractive & repulsive forces somehow analogous in molecular & atomic interactions as well.**

- **Most biological molecules** are made up of combinations of **six vital elements,** whose chemical symbols are **CHNOPS**.



- **CHNOPS**: Carbon, Hydrogen, Nitrogen, Oxygen, Phosphorus, and Sulfur
- Around 99.3% of all total number of atoms in **living organism** is composed of:




THE HUMAN BODY
ELEMENTAL COMPOSITION BY MASS
HYDROGEN
PERCENT 10
SYMBOL H
ATOMIC № 1
CARBON
PERCENT 18
SYMBOL C
ATOMIC № 6
NITROGEN
PERCENT 3
SYMBOL N
ATOMIC № 7
OXYGEN
PERCENT 65
SYMBOL O
ATOMIC № 8
FLUORINE
PERCENT <.01
SYMBOL F
ATOMIC № 9
SODIUM
PERCENT 0.1
SYMBOL Na
ATOMIC № 11
MAGNESIUM
PERCENT .05
SYMBOL Mg
ATOMIC № 12
PHOSPHORUS
PERCENT 1.2
SYMBOL P
ATOMIC № 6
SULFUR
PERCENT 0.2
SYMBOL S
ATOMIC № 16
POTASSIUM
PERCENT
SYMBOL K
CALCIUM
PERCENT
SYMBOL Ca
IRON
PERCENT
SYMBOL Fe
COBALT
PERCENT
SYMBOL Co

Geology

Astronomy

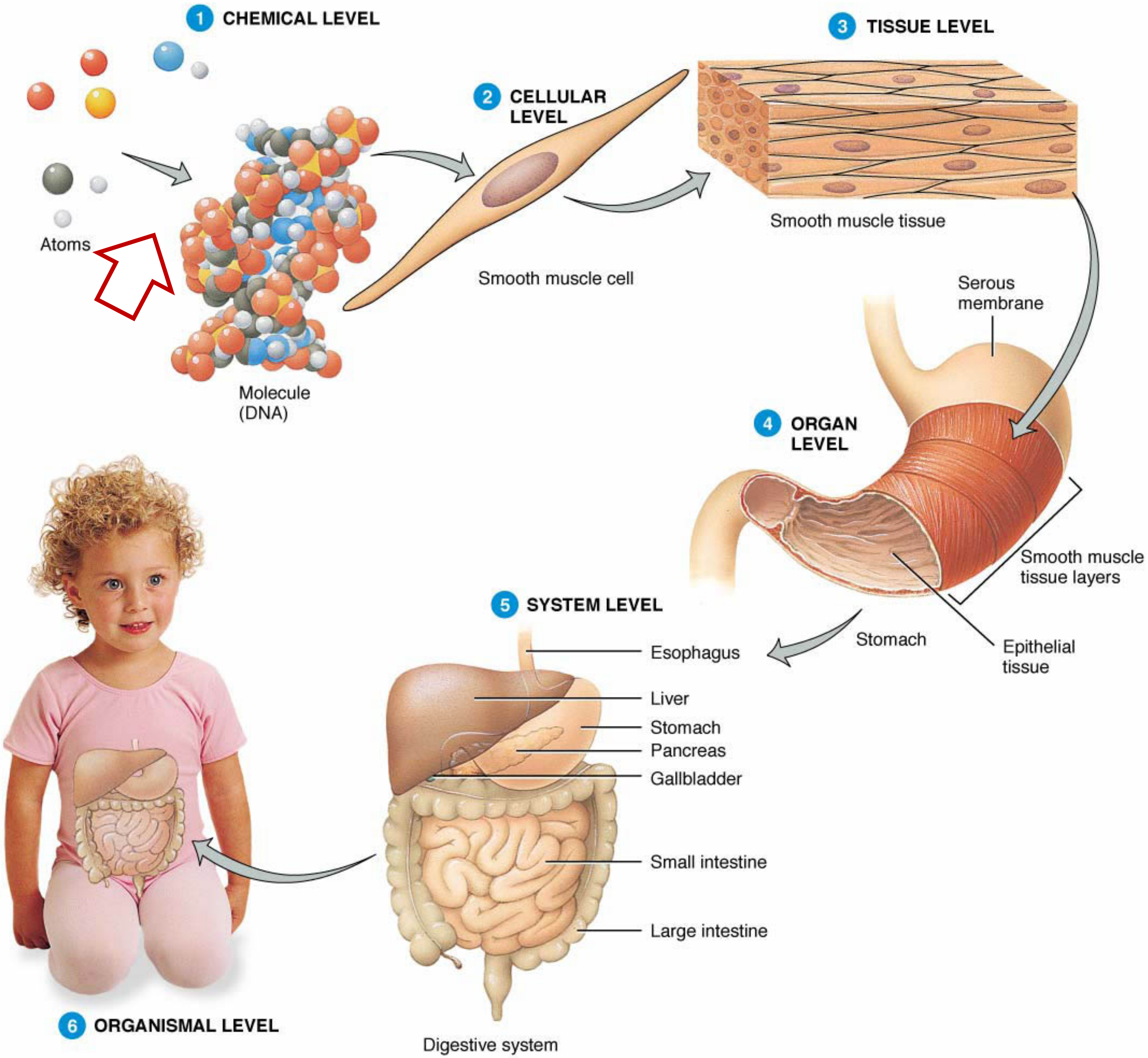
Weather & Climat

- However, it is **not merely** the composition of the atoms that **make up a system known as a living entity**.
- It is a:
  - Dynamic
  - Commucating
  - Growing
  - Renewing
  - Reproducing

  system that is **achieved** by **these elements** end up to be **living**.

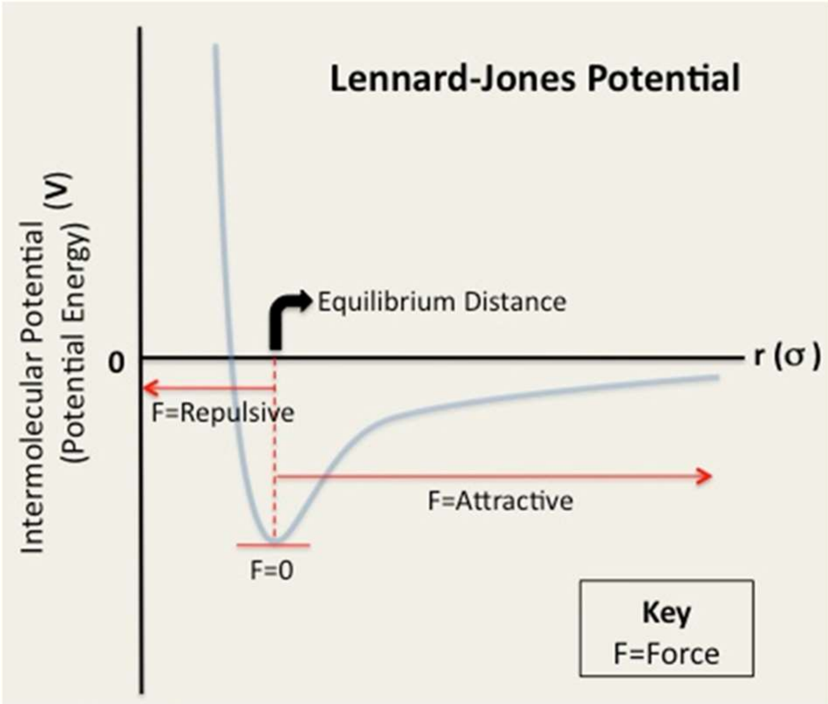
Essential Elements in the Human Body

Element	Percent by Mass*	Element
Oxygen	65	Sodium
Carbon	18	Magnesium
Hydrogen	10	Iron
Nitrogen	3	Cobalt
Calcium	1.6	Copper
Phosphorus	1.2	Zinc
Potassium	0.2	Iodine
Sulfur	0.2	Selenium



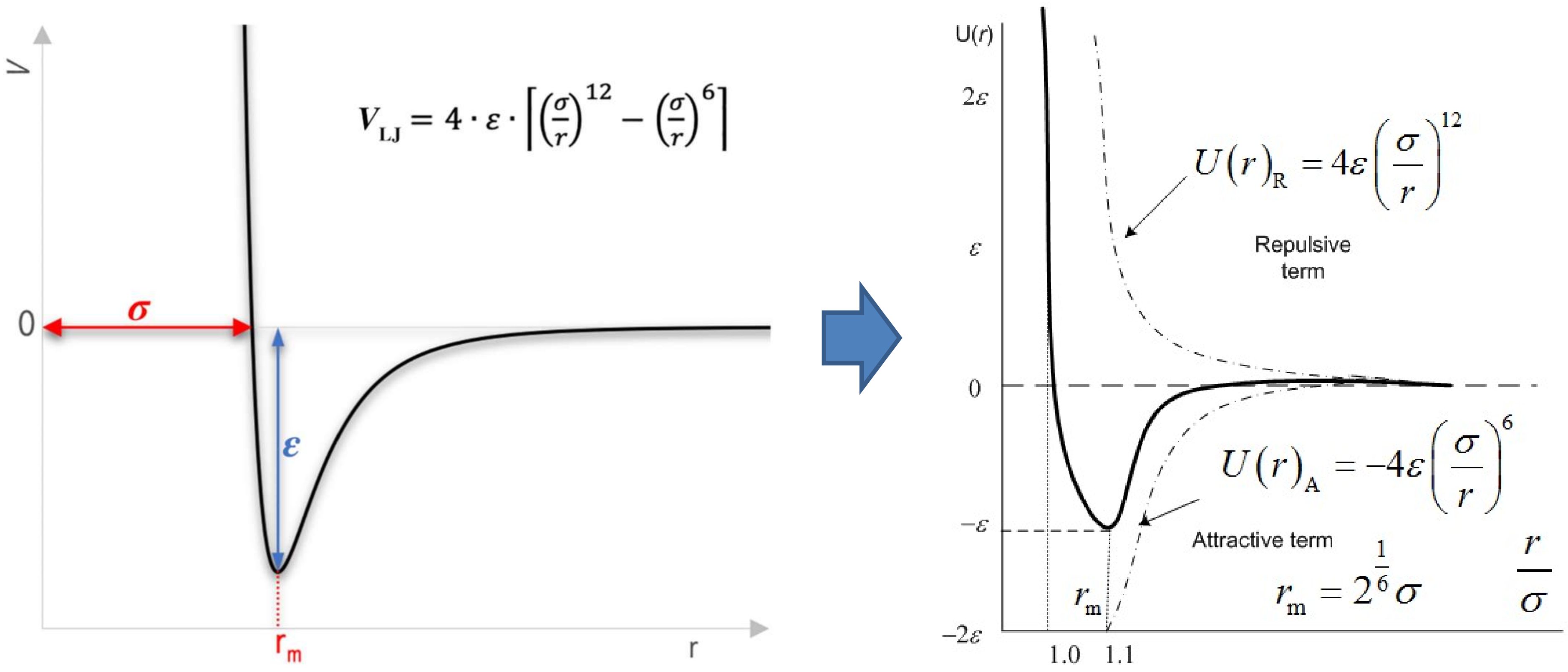
1 CHEMICAL LEVEL
Atoms
Molecule (DNA)
2 CELLULAR LEVEL
Smooth muscle cell
3 TISSUE LEVEL
Smooth muscle tissue
Serous membrane
4 ORGAN LEVEL
Smooth muscle tissue layers
Stomach
Epithelial tissue
5 SYSTEM LEVEL
Esophagus
Liver
Stomach
Pancreas
Gallbladder
Small intestine
Large intestine
Digestive system
6 ORGANISMAL LEVEL

The Bond Energy (AKA: Lennard-Jones Pot.)



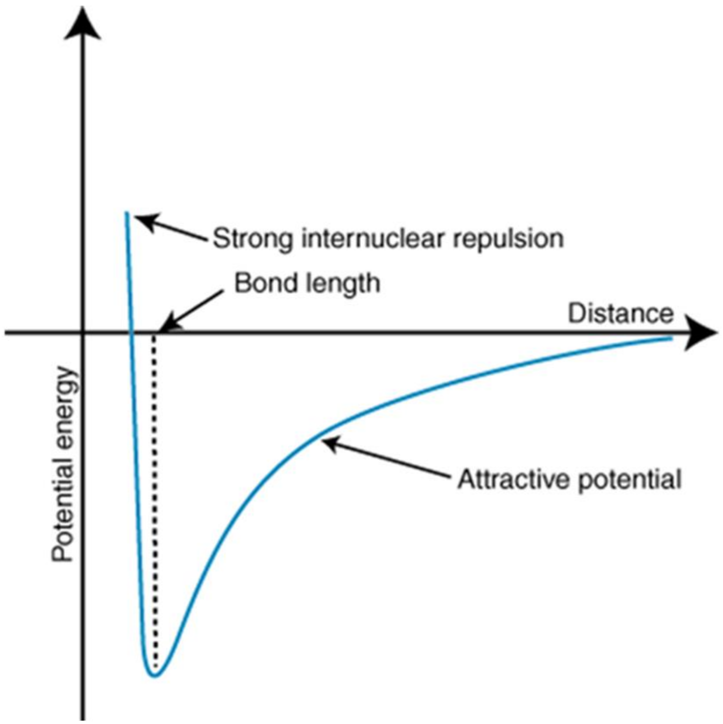
- Is a measure of a **chemical bond's strength** that is determined by measuring **the heat required to break one mole of molecules into their individual atoms**.

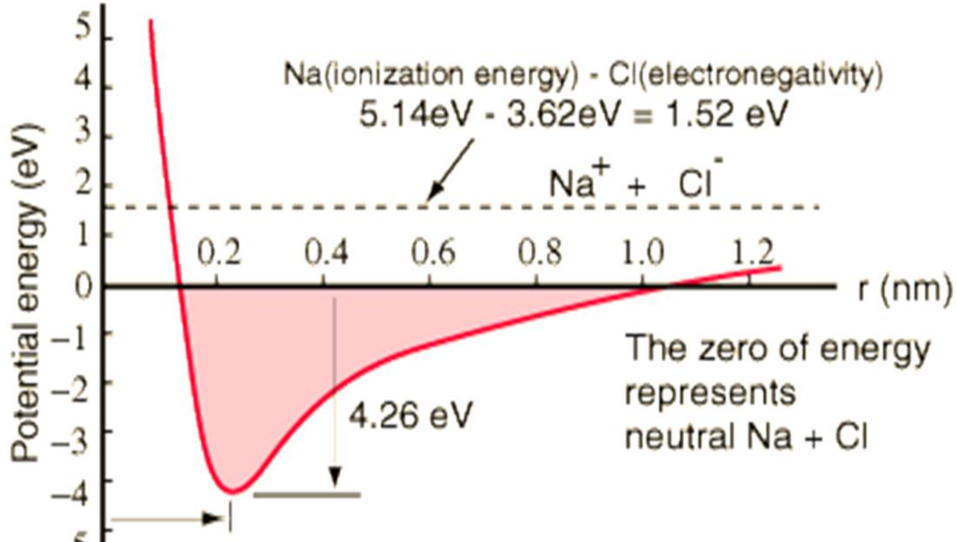
- Can be thought of as a **measure of the stability gained** when **two atoms bond to each other, as opposed to their free or unbound states**.



where

- V is the intermolecular potential between the two atoms or molecules.
- ϵ is the well depth and a measure of how strongly the two particles attract each other.
- σ is the distance at which the intermolecular potential between the two particles is zero (Figure 1). σ gives a measurement of how close two nonbonding particles can get and is thus referred to as the *van der Waals radius*. It is equal to one-half of the internuclear distance between nonbonding particles.
- r is the distance of separation between both particles (measured from the center of one particle to the center of the other particle).





1 eV = 1.60217662 × 10^{-19} J

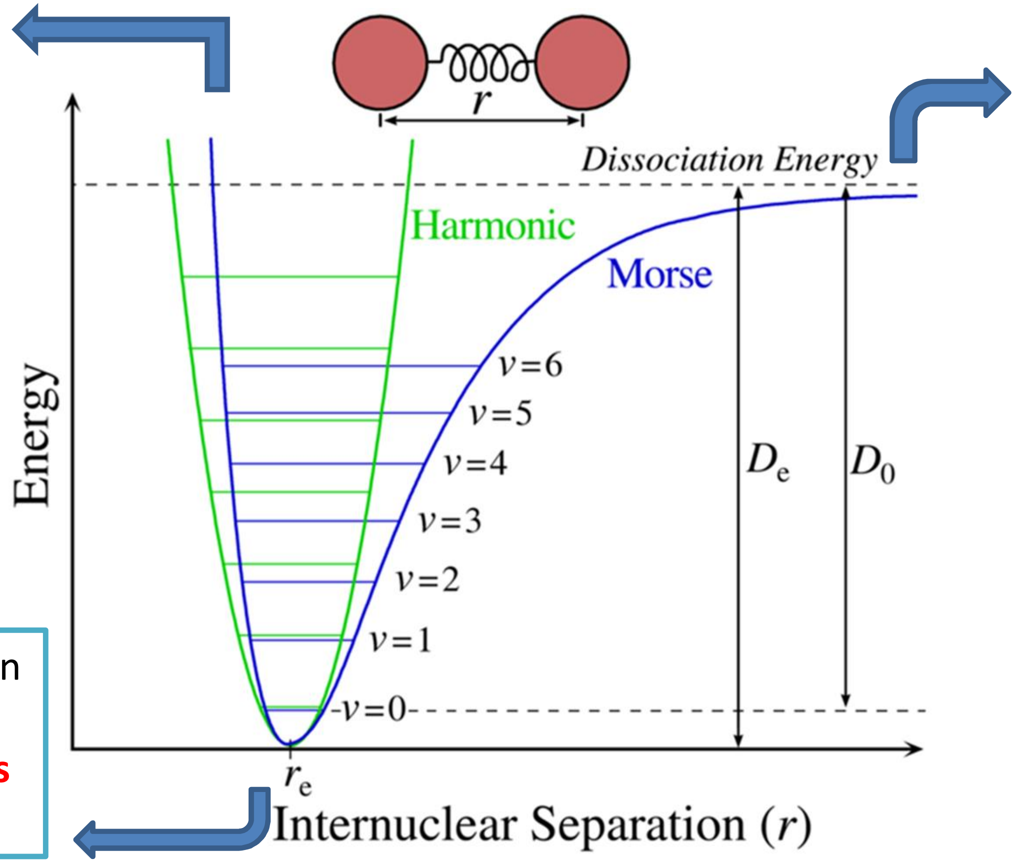
- Represents the **average energy** associated with **breaking the individual bonds of a molecule.**
- The **higher the bond energy** is, the "**stronger bond**" **occurs between the two atoms.**
  - The distance between them (bond length) is smaller.

A **Morse curve** shows **how the energy of a two atomic systems change as a function of internuclear distance.**

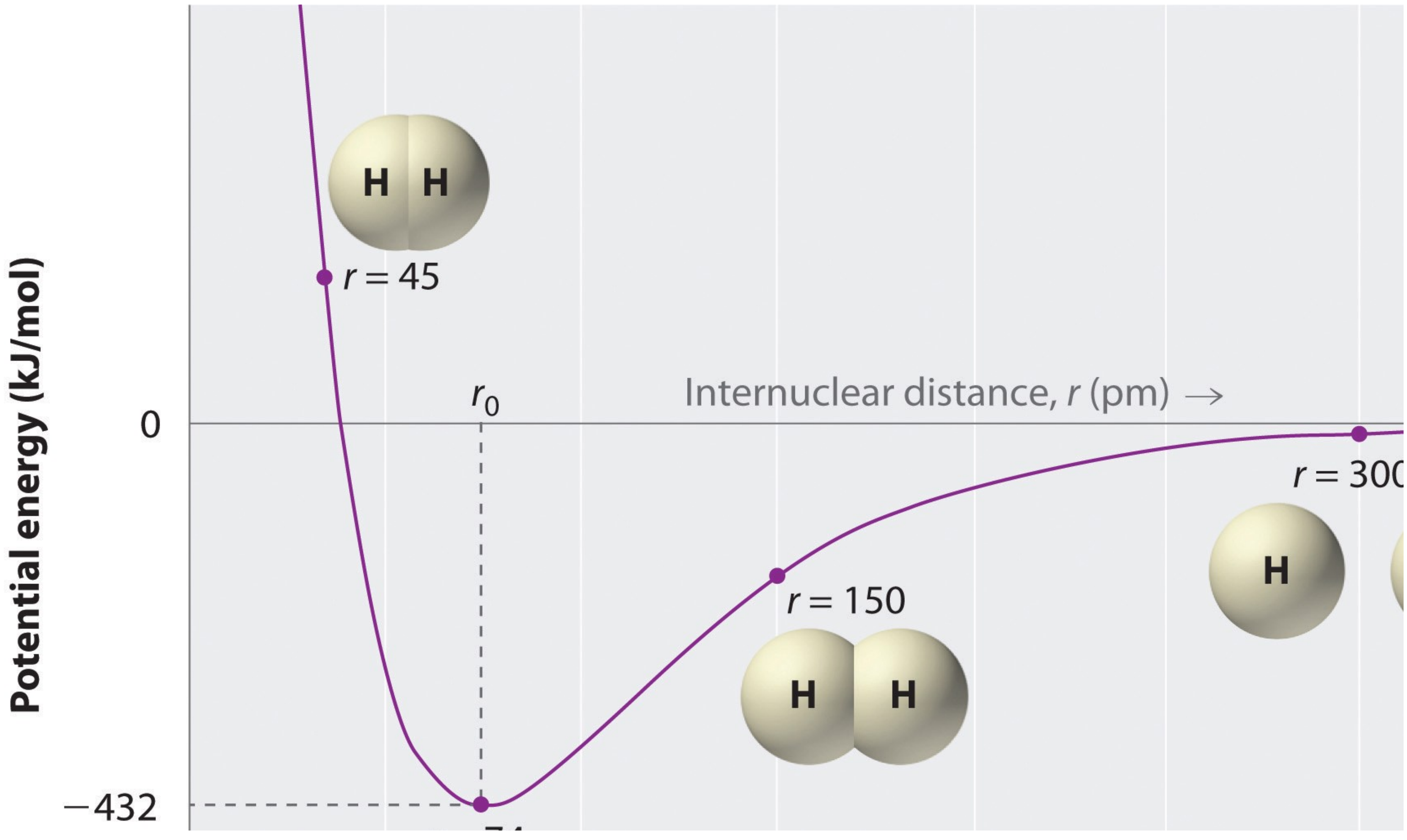
At very small distances between the two atoms, **the force is repulsive** and the energy of the two atom system is very high.

At large distances, the energy is zero, meaning that there is **no interaction**.

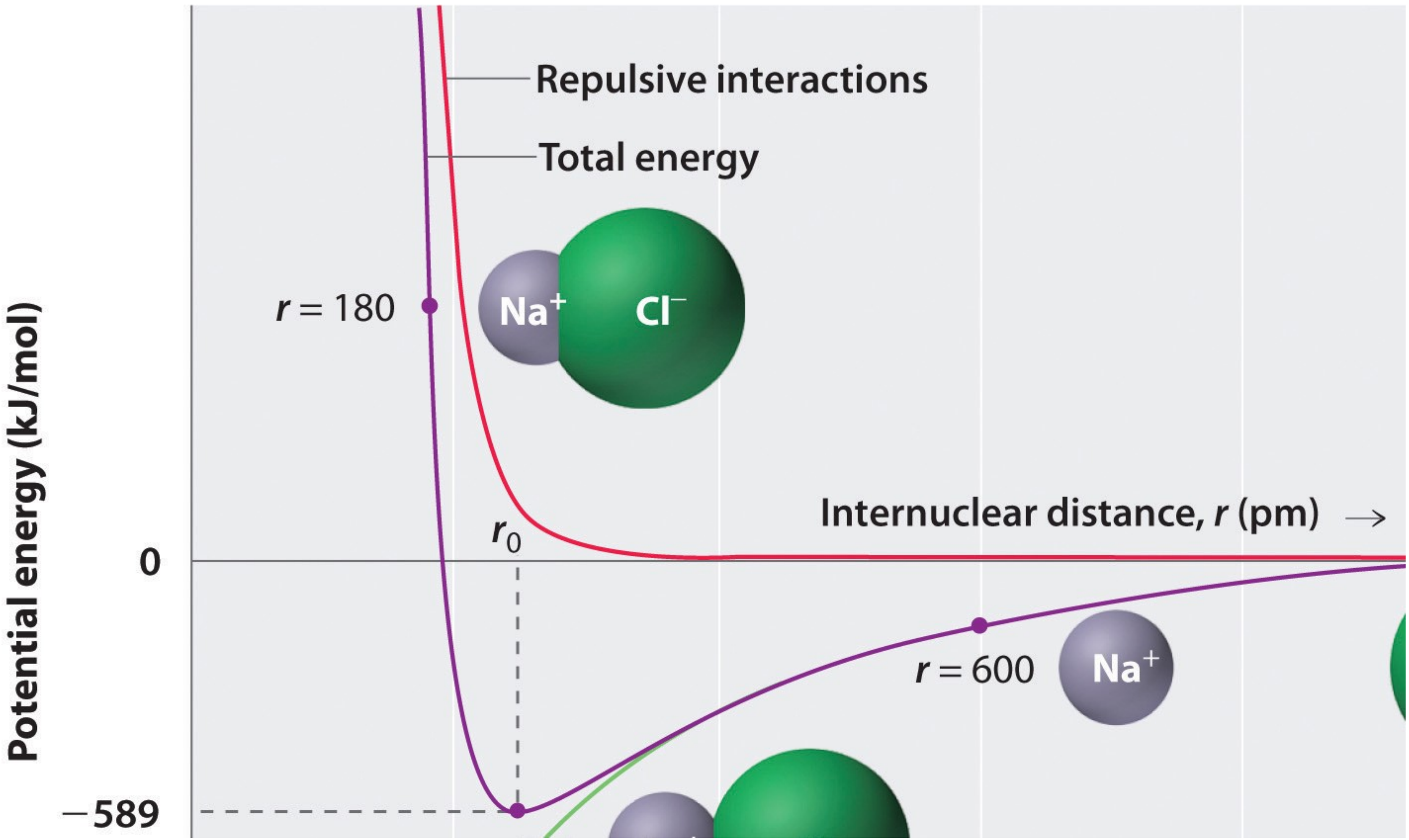
At internuclear distances in the order of an atomic diameter, **attractive forces dominate.**



Morse curve: Plot of potential energy vs distance between two atoms. The bond energy is energy that must be added from the minimum of the 'potential energy well' to the point of zero energy, which represents the two atoms being infinitely far apart, or, practically speaking, not bonded to each other.

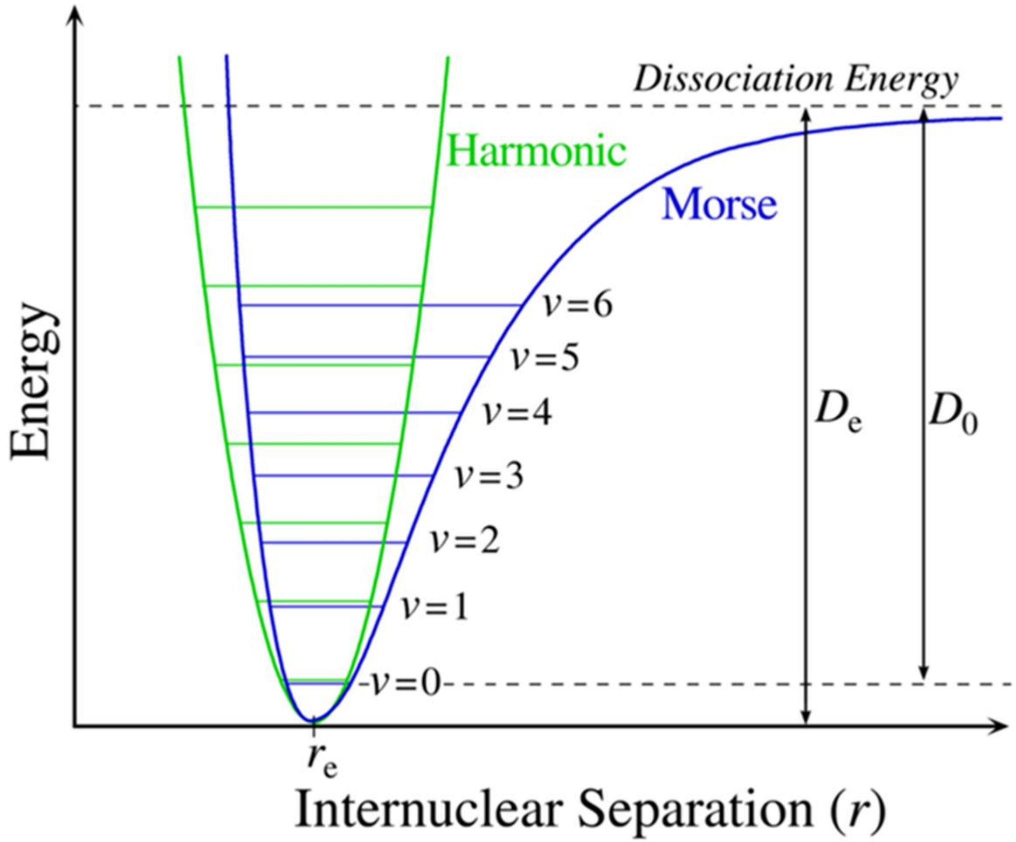


Potential energy (kJ/mol)
0
−432
r = 45
H H
r0
Internuclear distance, r (pm) →
r = 150
H H
H

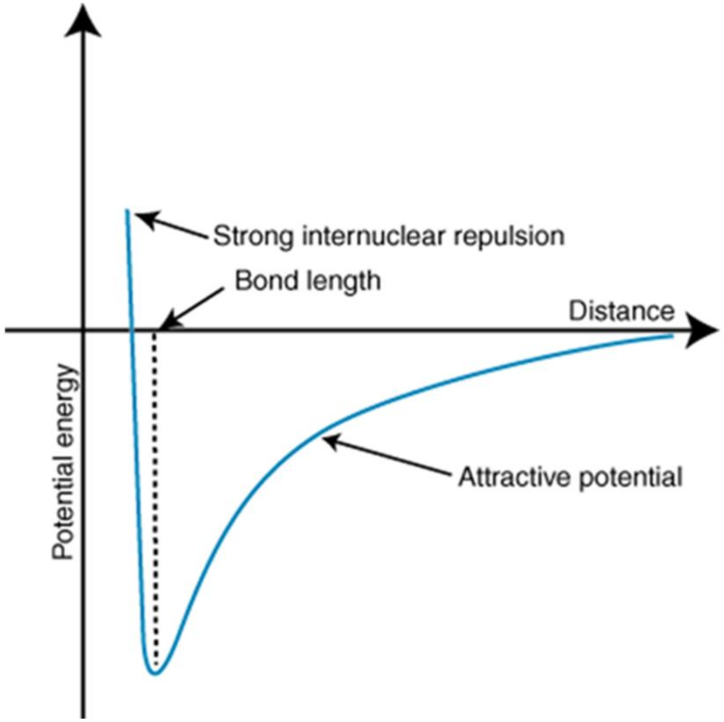


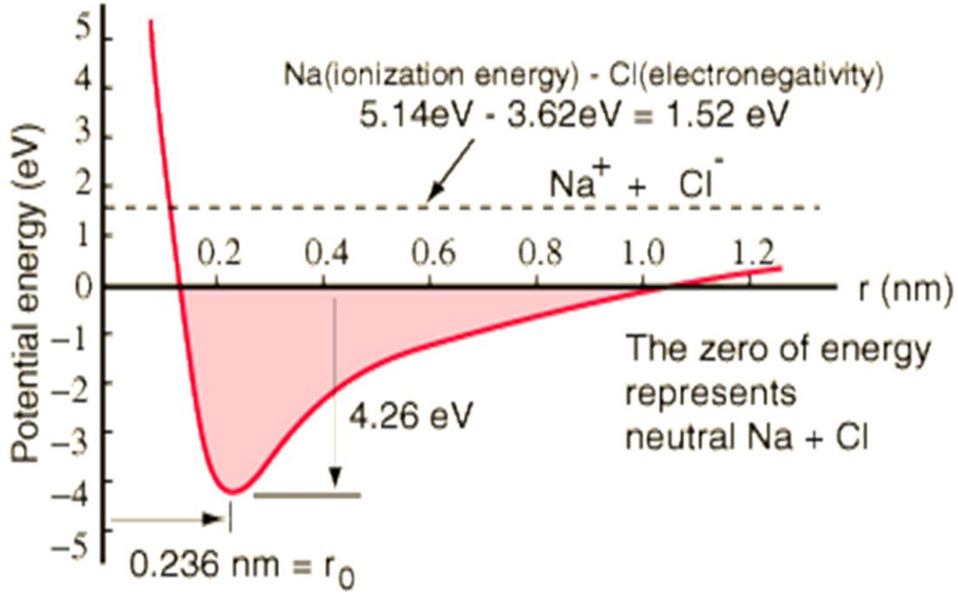
Repulsive interactions
Total energy
r = 180
Na+
Cl−
Internuclear distance, r (pm) →
r0
0
r = 600
Na+
−589
Potential energy (kJ/mol)

The **attractive** and **repulsive** **forces** are balanced at a minimum point in the plot of a **Morse curve.**



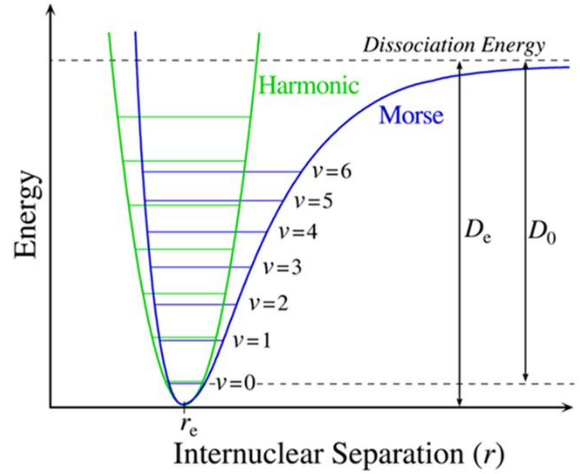
The **internuclear distance** at which the **energy minimum** occurs **defines** the **equilibrium bond length**.

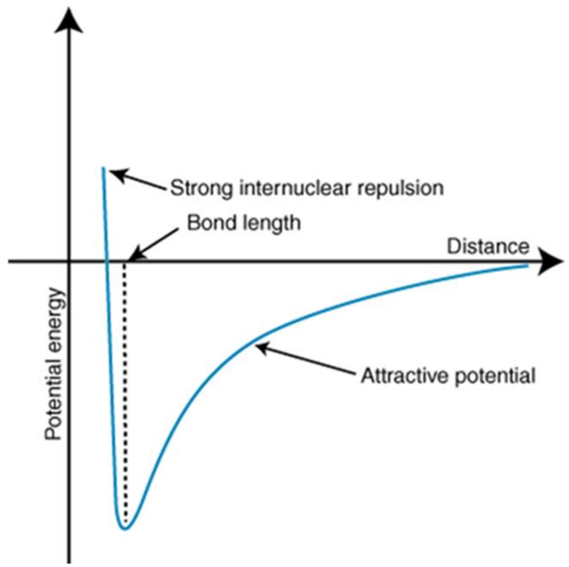


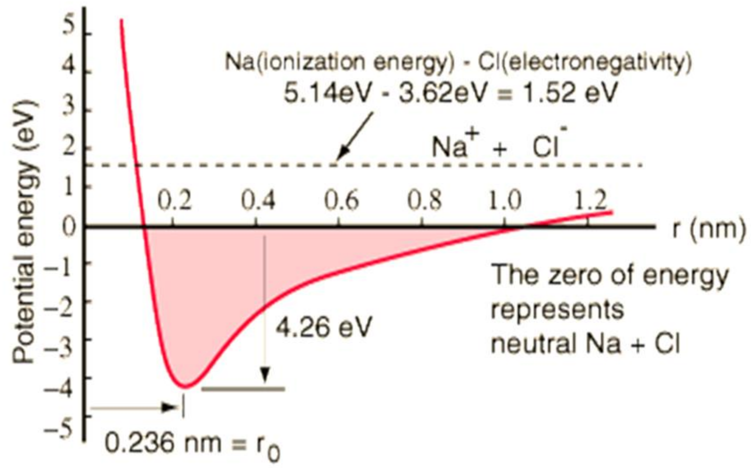


- The **bond length** represents an '**equilibrium**' value (because thermal motion causes the two atoms to vibrate about this distance, much like a spring vibrates back and forth around its unstretched, or equilibrium distance.)

In general, **stronger the bond** between two atoms, **the lower the energy minimum is** and **the smaller the bond length.**



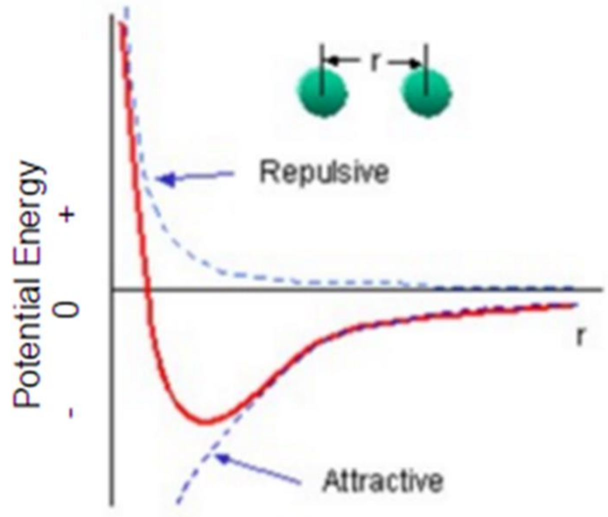




- Attractive forces (F_A)

$$F_A \propto \frac{1}{r^n}$$

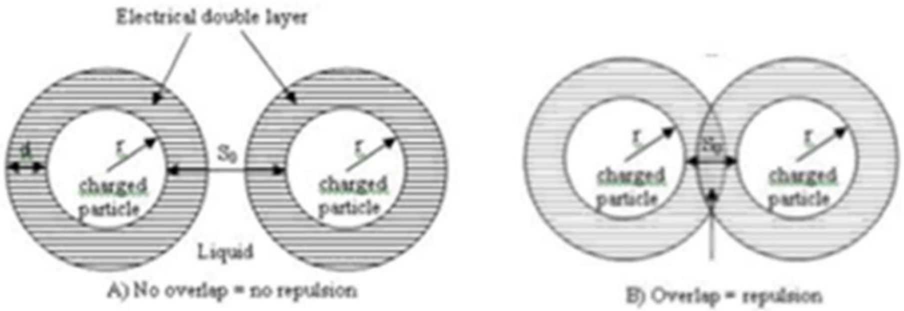
  - long range interaction
  - n= ~6 or 7 for H, N, ~3 or 4 for Cl
  - Cohesive : btw same molecules
  - Adhesive : btw different molecules



- Repulsive forces (F_R)

$$F_R \propto e^{1/r}$$

  - short range interaction
  - electron clouds interact

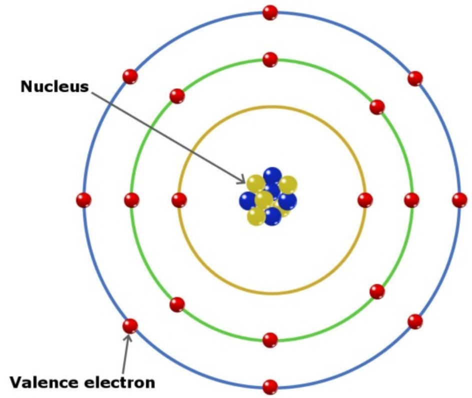


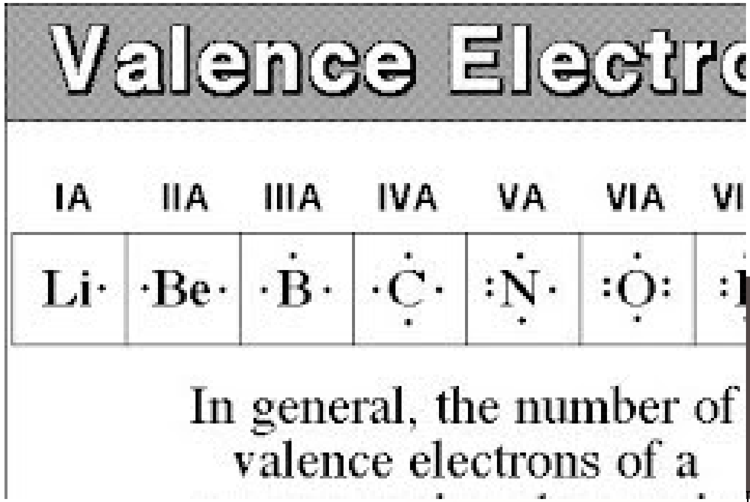
Valance Electrons & The Octet Rule

- **Matter always wants to be in the most stable form.**
- For any atom, **stability is achieved by following** "**octet rule**", which is to **say all atoms** (with a few exceptions) **want 8 electrons** in their **outermost electron shell.**
- The **electrons present in the outermost shell of an atom** are called "**valence electrons**".
- **Exceptions to the octet rule** include **hydrogen (H) and helium (He)** that follow **the duet rule** instead.
  - They have a single electron shell which accommodates only 2 electrons.

Boron Hydride (Borane)

group	number of electrons	number of bonds	examples
column 1	duet (2)	1	H_2, LiH
column 2	quartet (4)	2	BeH_2 , MgI_2
column 3	sextet (6)	3	BH_3 , $AlCl_3$
columns 4-8	octet (8)	4 bonds 3 bonds + 1 lone pair 2 bonds + 2 lone pairs 1 bond + 3 lone pairs	CH_4 NH_3 H_2O HCl





VALENCE ELECTRONS

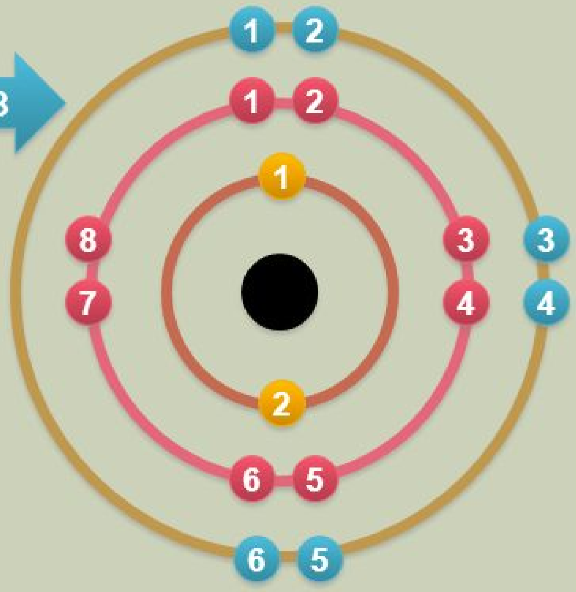
Valence Electron

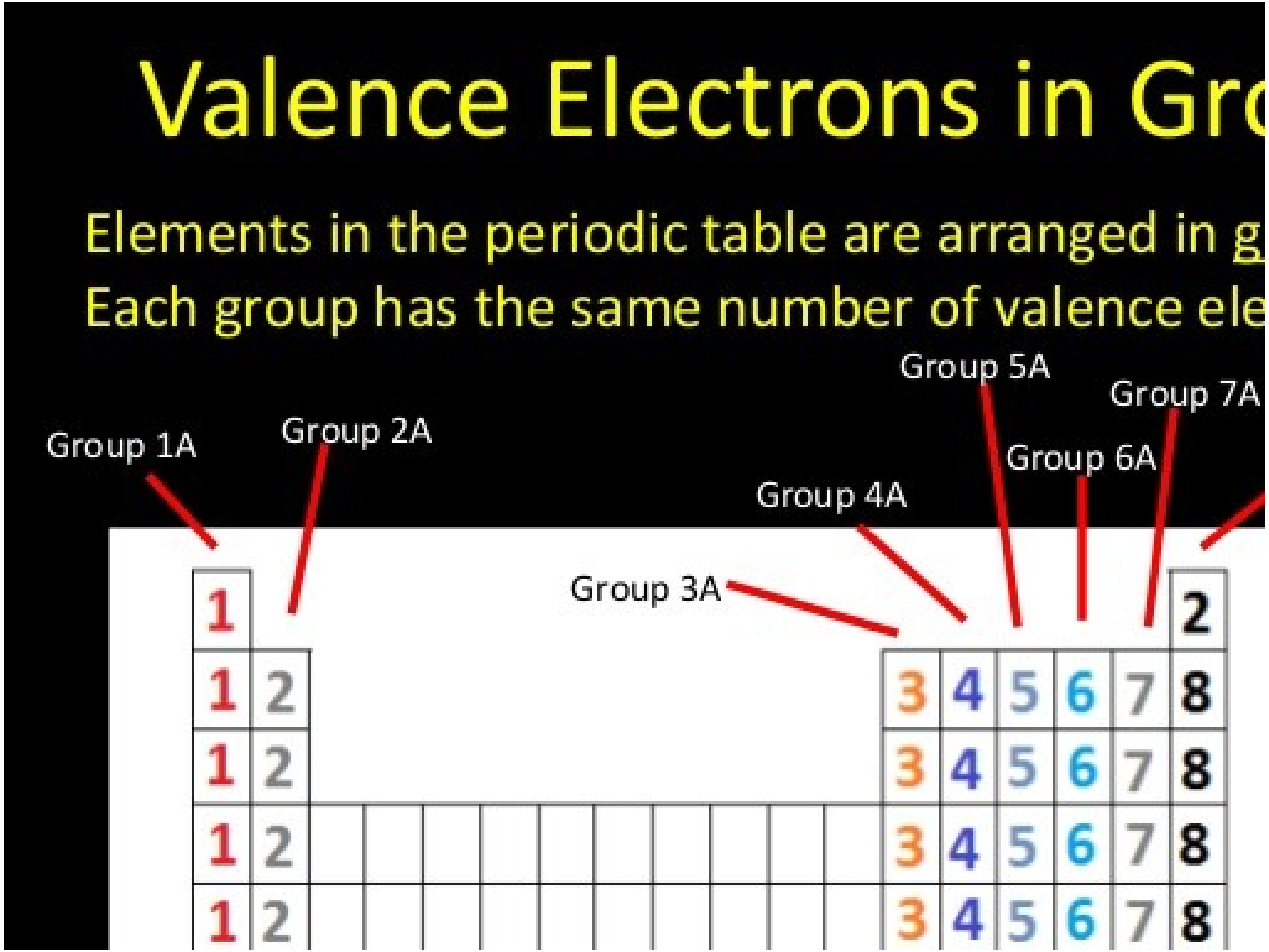
Valence electrons: electrons in the last shell or energy level of an atom.

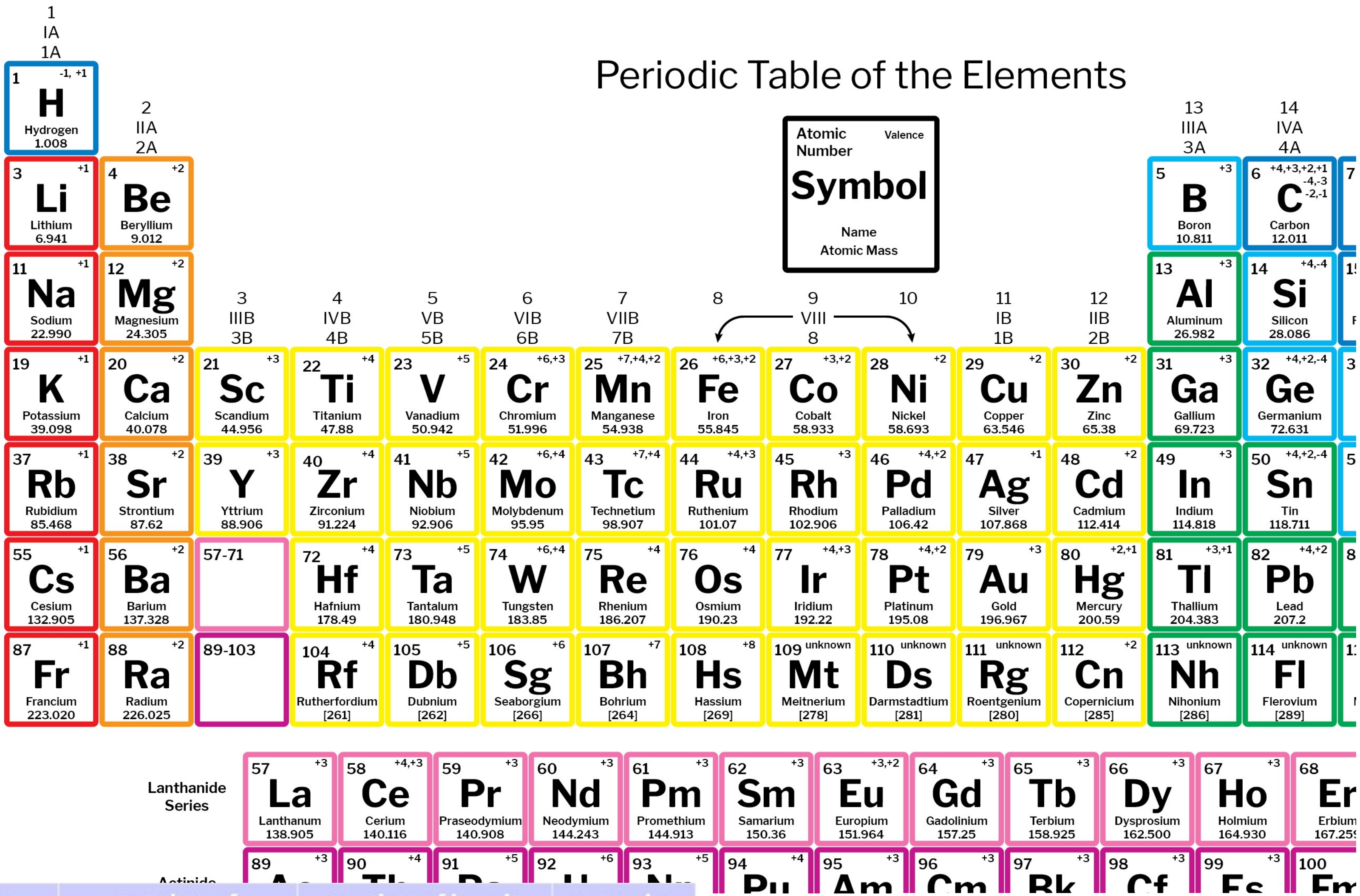
Last energy level: Level 3

So count the electrons in the last energy level

6 Valence Electrons!




Valence Electrons in Gro
Elements in the periodic table are arranged in g
Each group has the same number of valence ele
Group 1A
Group 2A
Group 3A
Group 4A
Group 5A
Group 6A
Group 7A
1
2
1 2 3 4 5 6 7 8
1 2 3 4 5 6 7 8
1 2 3 4 5 6 7 8
1 2 3 4 5 6 7 8



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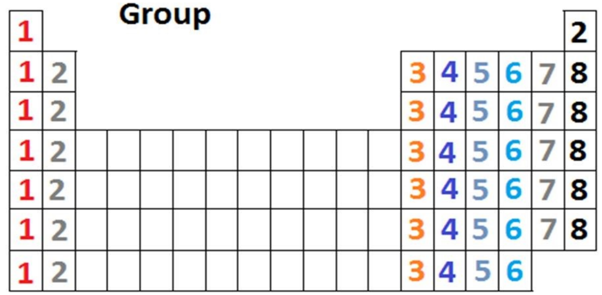
Valence Electrons in Each Group



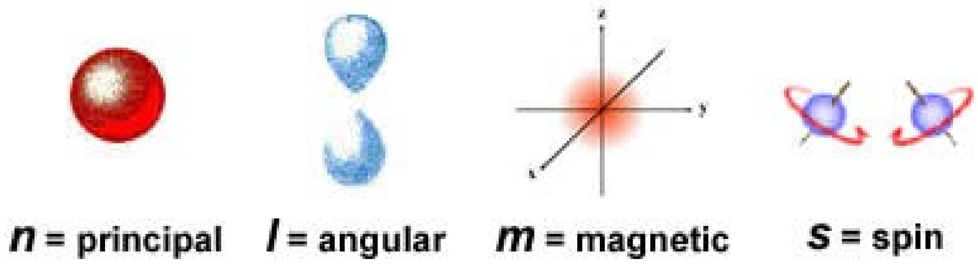
Quantum Mechanical Model & Atomic Orbital Concept

- The quantum mechanical model is based on quantum theory.

- **According to this theory**, it's **impossible to know** the **exact position** and **momentum of an electron at the same time**. This is known as the "**Uncertainty Principle**".

- Uses **complex shapes of orbitals** (electron clouds), **volumes of space** in which there is likely to be an **electron**. So, this model is based on **probability** rather than **certainty**.

- Four numbers, called **quantum numbers**, were introduced to **describe** the characteristics of **electrons and their orbitals**:

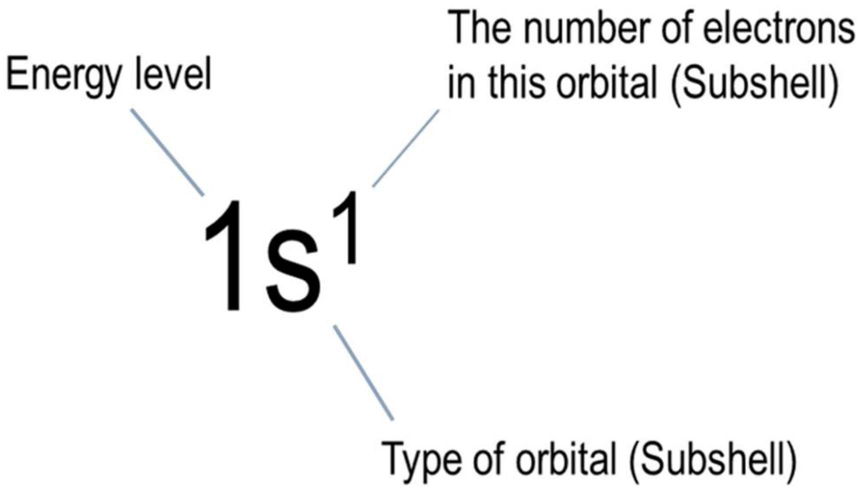


Symbol	Name	Values	Defines	Notes
n	principle	Positive integers (1, 2, 3 ...)	Electron shell (1=K, 2=L, 3=M, etc.)	Principle binding energy
l	azimuthal	Integers from 0 to $(n-1)$	Electron cloud shape (0=sphere, 1=dumbbell, etc.)	Orbital angular momentu optical spectroscopy conv rather than numbers: **sha** $(l = 1)$, **diffuse** $(l = 2)$, **fu**
m	magnetic	$-l$ to $+l$	Electron orientation in magnetic field	Not significant in the abse magnetic field

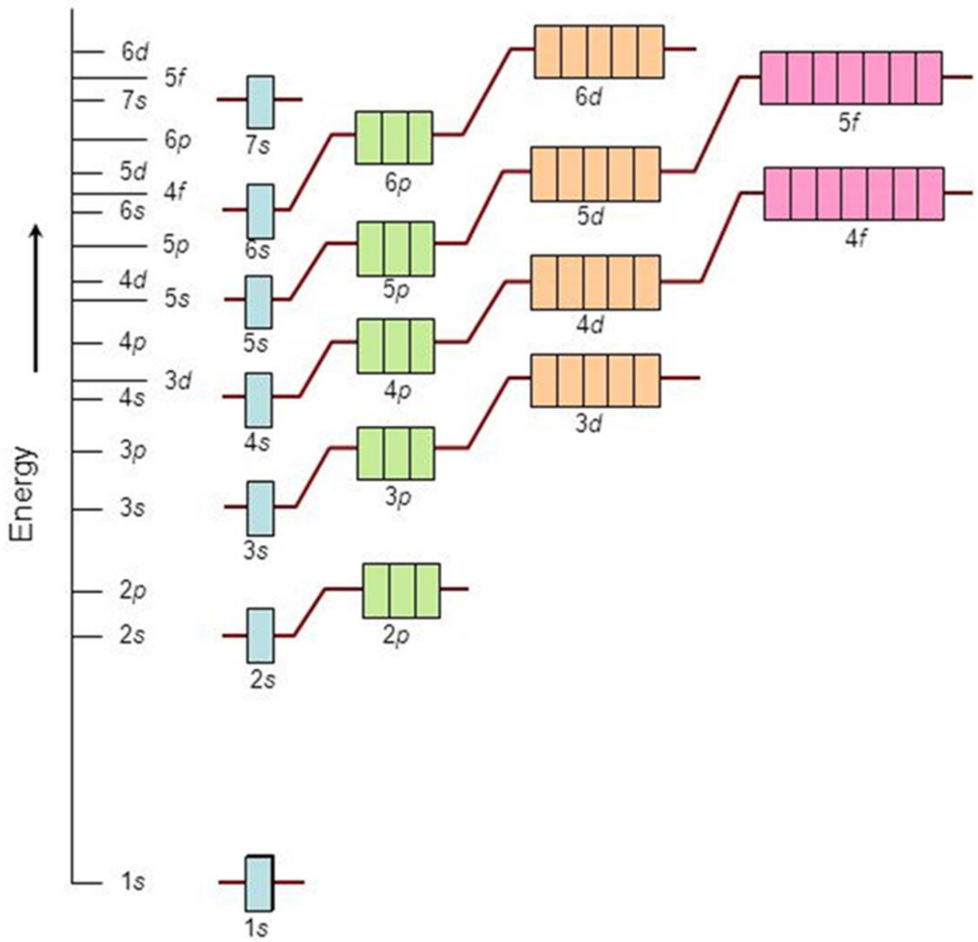
- **n describes the average distance of the orbital from the nucleus** — and the **energy** of the electron in an atom. **The larger the value of n is, the higher the energy and the larger the orbital**.
- ***l* describes the shape of the orbital**, and the shape is limited by the principal quantum number n.
  - Orbitals that have the same value of n but different values of "***l*** " are called "***subshells***".
- **m describes how the various orbitals are oriented in space**. The value of this number depends on the value of *l*.
- **s describes the direction the electron is spinning in a magnetic field** — either clockwise or counterclockwise.

Electron Configuration

- The arrengement of electrons in an atom is its electron configuration.
- Every element have a **unique electron configuration** because they all have different numbers of electron.

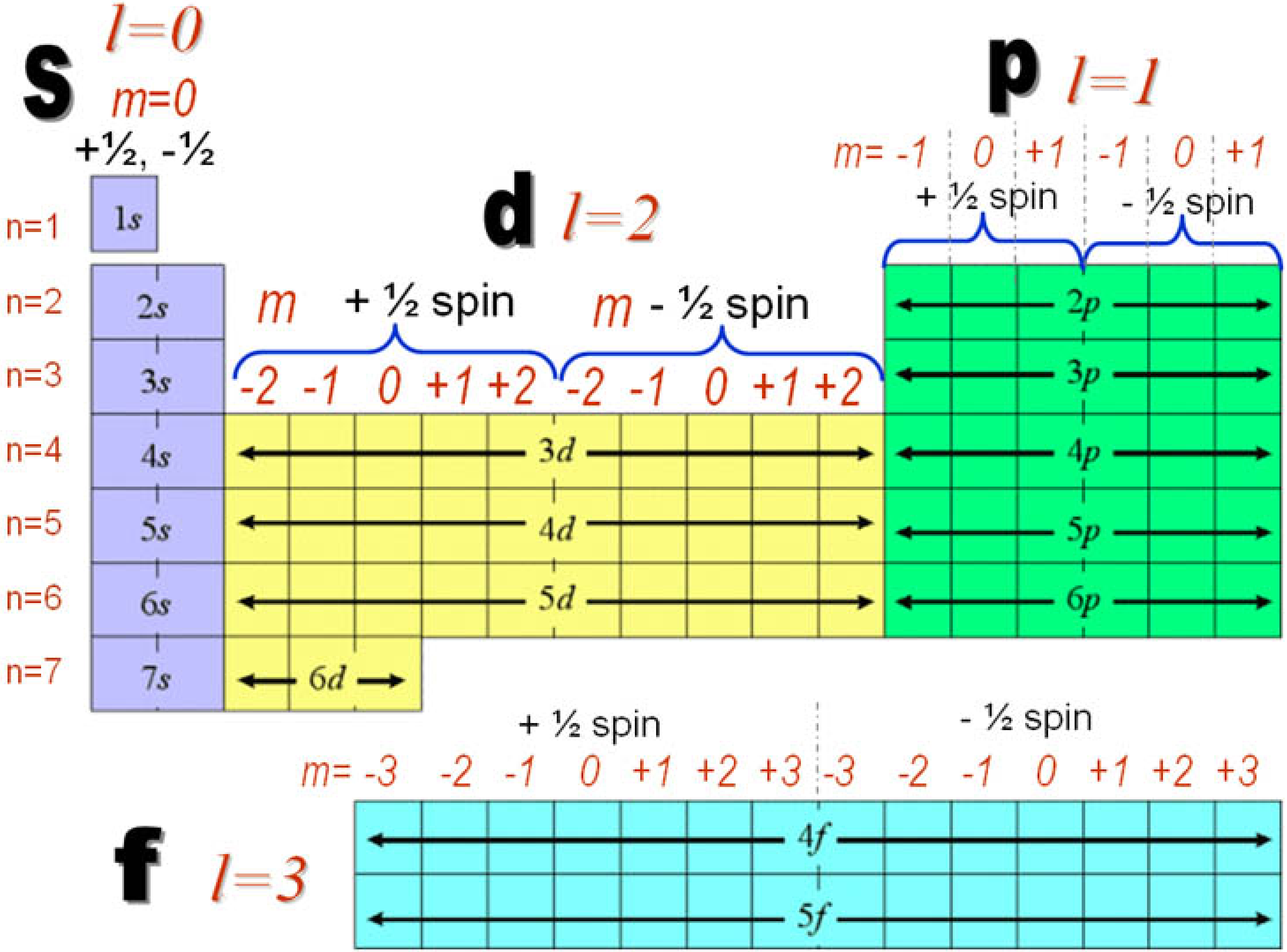


- K: $[Ar]4s^1$; $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$
- K^{+1}: $[Ar]$; $1s^2 2s^2 2p^6 3s^2 3p^6$
- P: $[Ne]3s^2 3p^3$; $1s^2 2s^2 2p^6 3s^2 3p^3$
- P^{-3}: $[Ne]3s^2 3p^6$; $1s^2 2s^2 2p^6 3s^2 3p^6$
- Al: $[Ne]3s^2 3p^1$; $1s^2 2s^2 2p^6 3s^2 3p^1$
- Al^{+3}: $[Ne]$; $1s^2 2s^2 2p^6$
- Se: $[Ne]4s^2 3d^{10} 4p^4$; $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^4$
- Se^{-2}: $[Ne]4s^2 3d^{10} 4p^6$; $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6$

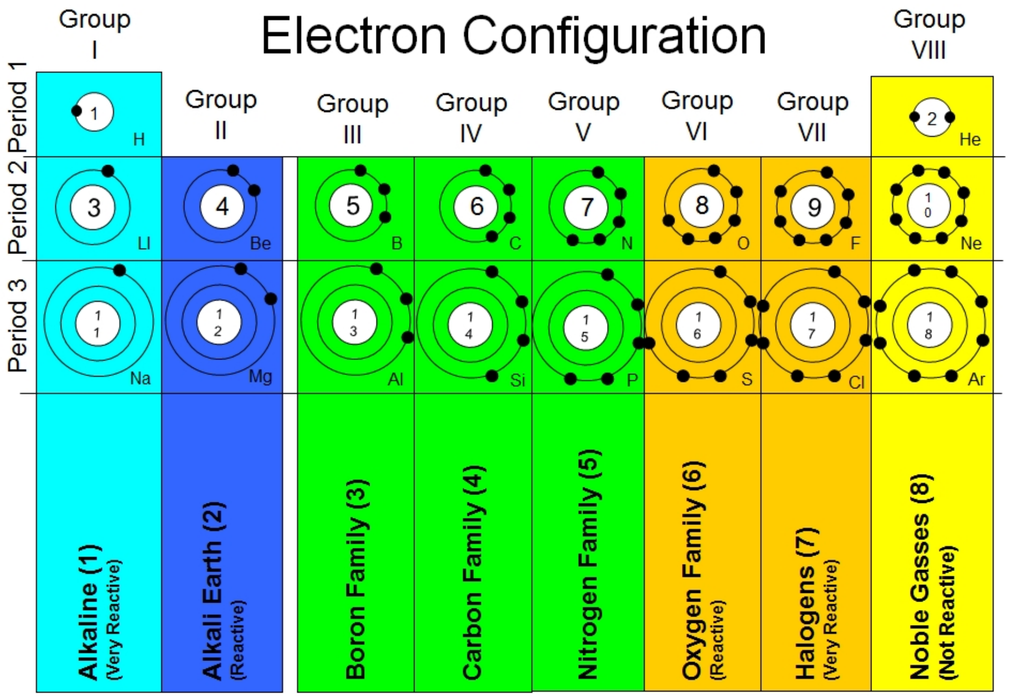


Atom Structure - Electrons

Sub-shell Type	# Sub-shells/ Shell	# Electrons / Full Sub-shell
s	1	2
p	3	6 (2 x 3)
d	5	10 (2 x 5)
f	7	14 (2 x 7)


s
l=0
m=0
+½, -½
p l=1
m= -1 0 +1 -1 0 +1
+ ½ spin
- ½ spin
d l=2
m + ½ spin
m - ½ spin
-2 -1 0 +1 +2 -2 -1 0 +1 +2
n=1
n=2
n=3
n=4
n=5
n=6
n=7
1s
2s
3s
4s
5s
6s
7s
3d
4d
5d
6d
2p
3p
4p
5p
6p
+ ½ spin
- ½ spin
m= -3 -2 -1 0 +1 +2 +3 -3 -2 -1 0 +1 +2 +3
f l=3
4f
5f

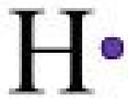
Atoms	Electronic Configuration	Lewis Symbol
sodium	$[Ne]3s^1$	Na •
magnesium	$[Ne]3s^2$	• Mg •
aluminum	$[Ne]3s^2 3p^1$	• Al • (with one dot above)
silicon	$[Ne]3s^2 3p^2$	• Si • (with one dot above and one below)
phosphorus	$[Ne]3s^2 3p^3$	• P • (with two dots above and one below)
sulfur	$[Ne]3s^2 3p^4$	: S • (with two dots above and one below)
chlorine	$[Ne]3s^2 3p^5$	: Cl • (with two dots above and two below)
argon	$[Ne]3s^2 3p^6$	: Ar : (with two dots above and two below)



Drawing Lewis structures

1. Calculate the total number of valence electrons in the compound.
2. Choose the central atom and place the remaining atoms symmetrically around the central atom.
3. Place one electron pair (or a line) between each pair of bonded atoms.
4. Complete the octet of each atom (duplet for H) by placing the remaining valence electron as electron pairs around the atoms.

Let's examine the compound hydrogen chloride, HCl. First let's draw the Lewis Dot structure of hydrogen:

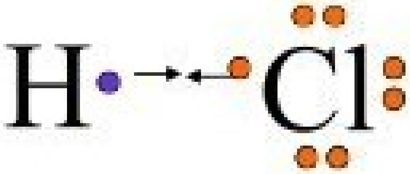


Hydrogen is in the first column so gets one dot to represent its one valence electron.

Now let's draw the Lewis Dot structure of chlorine:

Chlorine is in the seventh column so gets seven valence electrons.

We must now remember that most atoms will be stable when they have 8 valence electrons; a full octet. Hydrogen will be stable with only 2 electrons. We can now combine these two atoms together to form a covalent bond; sharing their electrons:



Hydrogen now has two valence electrons and is stable. Chlorine now has 8 valence electrons and is stable. By sharing their electrons, the atoms have managed to satisfy each others' valence shell to make a stable compound.

Drawing Lewis Structures

Example 1 - CCl_4

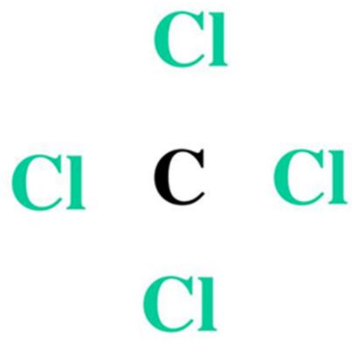
Step 1 - Determine the total # of valence shell electrons (e^{1-}) used.

C is in group 4, Cl is in group VII

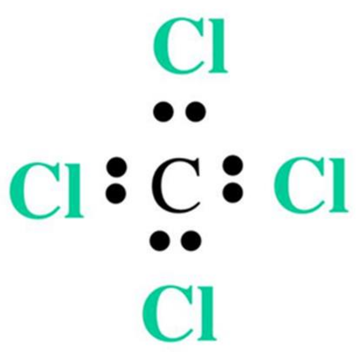
((4x 1) + (7x4)) = 32 e^{1-}

1 C atom in CCl_4 **4 Cl atoms in CCl_4**

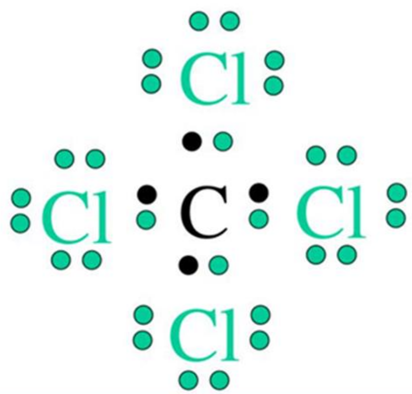
Step 2 - Place the single atom of C in the centre and place the 4 Cl atoms around it.



Step 3- Place a pair of electrons between each pair of atoms.



Step 4 - Place 8 electrons around all non-central atoms.

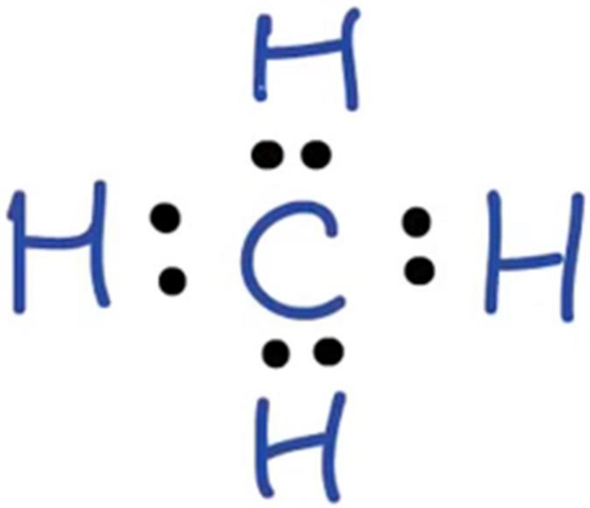


Step 1

Find the total number of valence electrons.

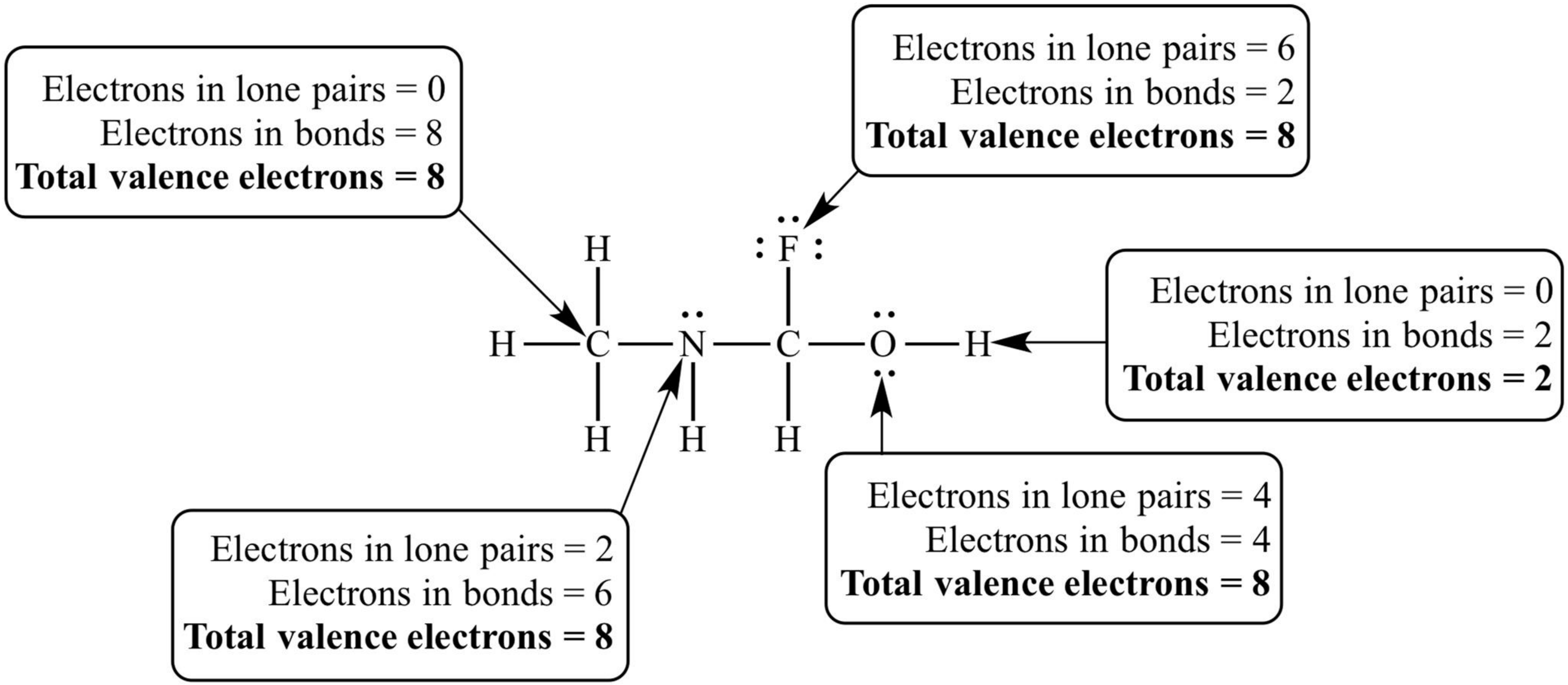
$$\text{Formal Charge} = \text{Valence Electrons} - \text{NonBonding Val Electrons} - \frac{\text{Bonding Electrons}}{2}$$

Formal Charges



$$\text{Formal Charge} = \text{Valence Electrons} - \text{NonBonding Val Electrons} - \frac{\text{Bonding Electrons}}{2}$$

- Formal charges **allow us to figure out which is going to be the best structure** for a chemical compound.


Electrons in lone pairs = 0
Electrons in bonds = 8
Total valence electrons = 8
Electrons in lone pairs = 6
Electrons in bonds = 2
Total valence electrons = 8
Electrons in lone pairs = 0
Electrons in bonds = 2
Total valence electrons = 2
Electrons in lone pairs = 2
Electrons in bonds = 6
Total valence electrons = 8
Electrons in lone pairs = 4
Electrons in bonds = 4
Total valence electrons = 8
H
C
N
C
O
H
F
H
H
H
H

Intramolecular Forces

Holds atoms together in a molecule

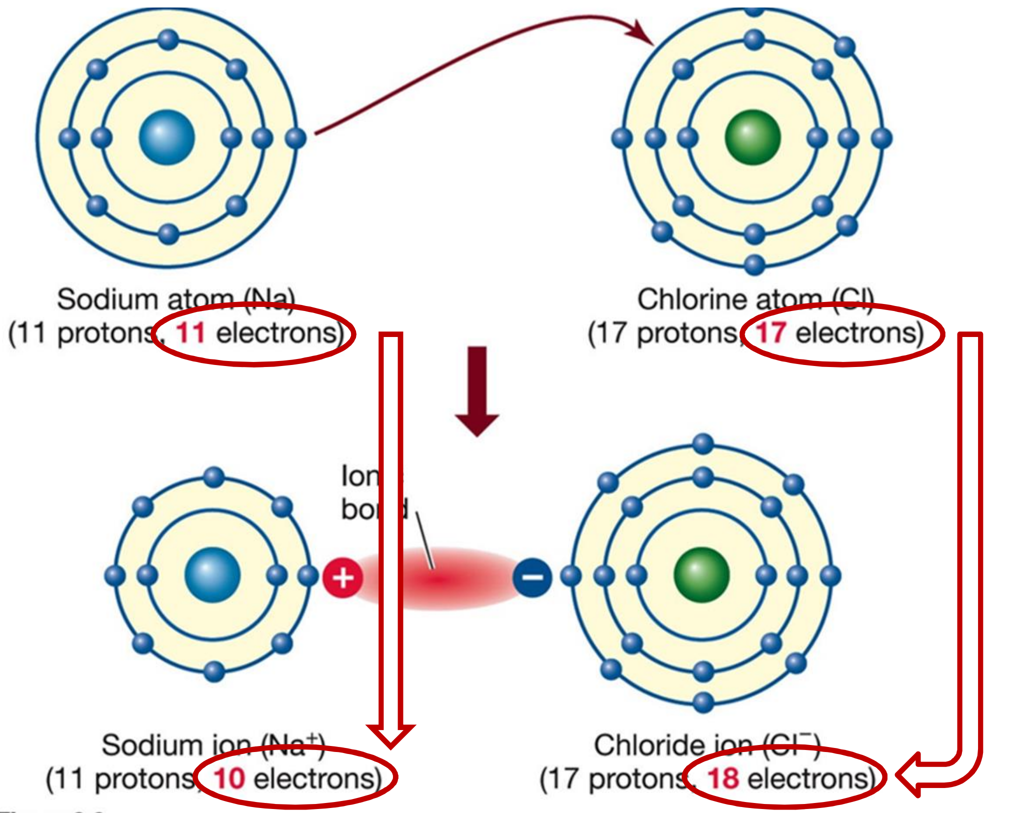
- Ionic Bonding
- Covalent Bonding
- Metallic Bonding

Intramolecular Forces

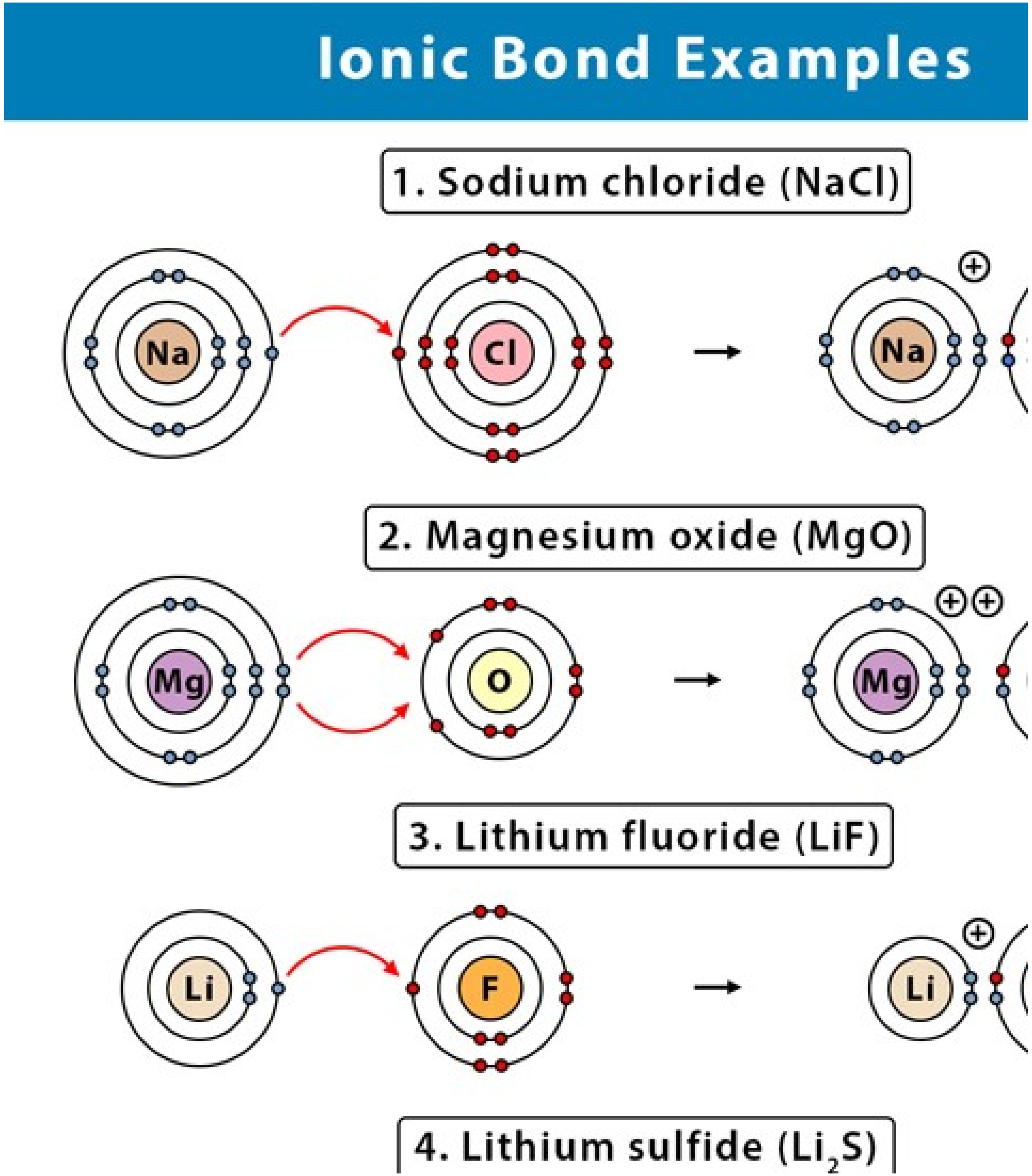
- **Ionic Bonding**
  - Is formed by the **complete transfer of valence electron(s) between atoms**.
  - The metal loses electrons to become a positively charged cation, whereas the non-metal accepts those electrons to become a negatively charged anion.

In biological environment;
✓ B/t ionizable groups of proteins and small ions
✓ B/t phosphate groups and cations in nucleic acids

*B/t: Between



LIFE 9e, Figure 2.9


Ionic Bond Examples
1. Sodium chloride (NaCl)
Na
Cl
Na
2. Magnesium oxide (MgO)
Mg
O
Mg
3. Lithium fluoride (LiF)
Li
F
Li
4. Lithium sulfide (Li_2S)

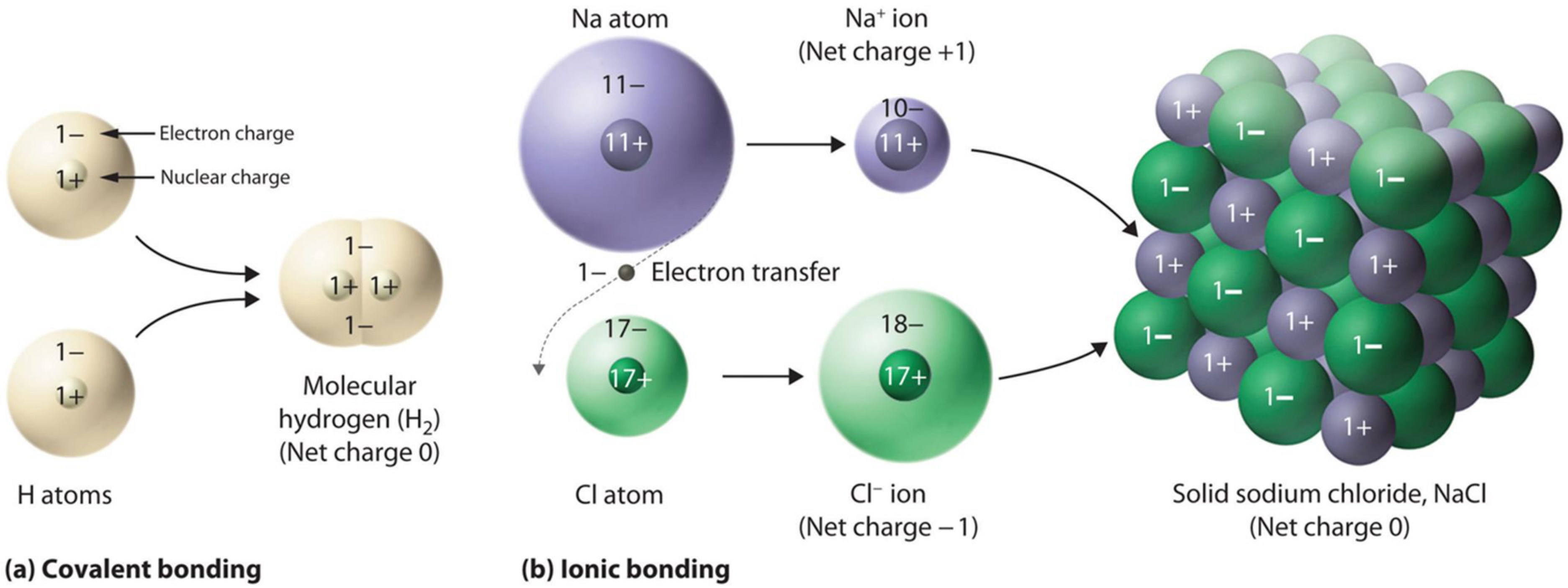
Periodic Table of the Elements

Atomic Number	Valence
Symbol	
Name	
Atomic Mass	

1 IA 1A	2 IIA 2A	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8 VIII 8	9 VIII 8	10 VIII 8	11 IB 1B	12 IIB 2B	13 IIIA 3A	14 IVA 4A
1 **H** Hydrogen 1.008 (-1, +1)													
3 **Li** Lithium 6.941 (+1)	4 **Be** Beryllium 9.012 (+2)											5 **B** Boron 10.811 (+3)	6 **C** Carbon 12.011 (+4,+3,+2,+1 -4,-3 -2,-1)
11 **Na** Sodium 22.990 (+1)	12 **Mg** Magnesium 24.305 (+2)											13 **Al** Aluminum 26.982 (+3)	14 **Si** Silicon 28.086 (+4,-4)
19 **K** Potassium 39.098 (+1)	20 **Ca** Calcium 40.078 (+2)	21 **Sc** Scandium 44.956 (+3)	22 **Ti** Titanium 47.88 (+4)	23 **V** Vanadium 50.942 (+5)	24 **Cr** Chromium 51.996 (+6,+3)	25 **Mn** Manganese 54.938 (+7,+4,+2)	26 **Fe** Iron 55.845 (+6,+3,+2)	27 **Co** Cobalt 58.933 (+3,+2)	28 **Ni** Nickel 58.693 (+2)	29 **Cu** Copper 63.546 (+2)	30 **Zn** Zinc 65.38 (+2)	31 **Ga** Gallium 69.723 (+3)	32 **Ge** Germanium 72.631 (+4,+2,-4)
37 **Rb** Rubidium 85.468 (+1)	38 **Sr** Strontium 87.62 (+2)	39 **Y** Yttrium 88.906 (+3)	40 **Zr** Zirconium 91.224 (+4)	41 **Nb** Niobium 92.906 (+5)	42 **Mo** Molybdenum 95.95 (+6,+4)	43 **Tc** Technetium 98.907 (+7,+4)	44 **Ru** Ruthenium 101.07 (+4,+3)	45 **Rh** Rhodium 102.906 (+3)	46 **Pd** Palladium 106.42 (+4,+2)	47 **Ag** Silver 107.868 (+1)	48 **Cd** Cadmium 112.414 (+2)	49 **In** Indium 114.818 (+3)	50 **Sn** Tin 118.711 (+4,+2,-4)
55 **Cs** Cesium 132.905 (+1)	56 **Ba** Barium 137.328 (+2)	57-71	72 **Hf** Hafnium 178.49 (+4)	73 **Ta** Tantalum 180.948 (+5)	74 **W** Tungsten 183.85 (+6,+4)	75 **Re** Rhenium 186.207 (+4)	76 **Os** Osmium 190.23 (+4)	77 **Ir** Iridium 192.22 (+4,+3)	78 **Pt** Platinum 195.08 (+4,+2)	79 **Au** Gold 196.967 (+3)	80 **Hg** Mercury 200.59 (+2,+1)	81 **Tl** Thallium 204.383 (+3,+1)	82 **Pb** Lead 207.2 (+4,+2)
87 **Fr** Francium 223.020 (+1)	88 **Ra** Radium 226.025 (+2)	89-103	104 **Rf** Rutherfordium [261] (+4)	105 **Db** Dubnium [262] (+5)	106 **Sg** Seaborgium [266] (+6)	107 **Bh** Bohrium [264] (+7)	108 **Hs** Hassium [269] (+8)	109 **Mt** Meitnerium [278] (unknown)	110 **Ds** Darmstadtium [281] (unknown)	111 **Rg** Roentgenium [280] (unknown)	112 **Cn** Copernicium [285] (+2)	113 **Nh** Nihonium [286] (unknown)	114 **Fl** Flerovium [289] (unknown)

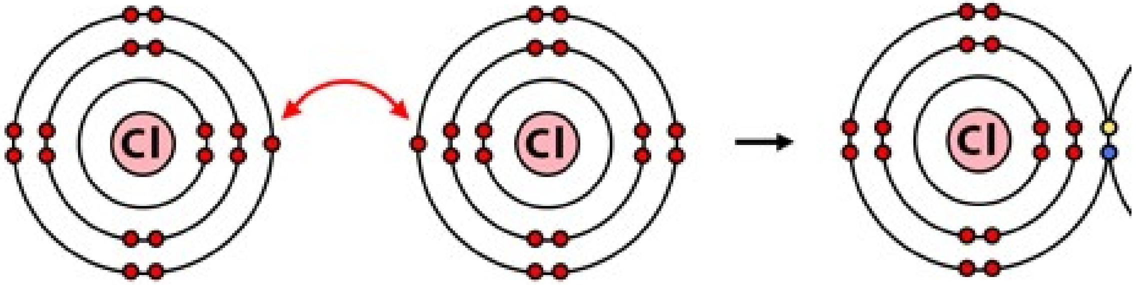
Series												
Lanthanide Series	57 **La** Lanthanum 138.905 (+3)	58 **Ce** Cerium 140.116 (+4,+3)	59 **Pr** Praseodymium 140.908 (+3)	60 **Nd** Neodymium 144.243 (+3)	61 **Pm** Promethium 144.913 (+3)	62 **Sm** Samarium 150.36 (+3)	63 **Eu** Europium 151.964 (+3,+2)	64 **Gd** Gadolinium 157.25 (+3)	65 **Tb** Terbium 158.925 (+3)	66 **Dy** Dysprosium 162.500 (+3)	67 **Ho** Holmium 164.930 (+3)	68 **Er** Erbium 167.25
Actinide	89 **Ac** (+3)	90 **Th** (+4)	91 **Pa** (+5)	92 **U** (+6)	93 **Np** (+5)	94 **Pu** (+4)	95 **Am** (+3)	96 **Cm** (+3)	97 **Bk** (+3)	98 **Cf** (+3)	99 **Es** (+3)	100 **Fm**

- ## Covalent Bonding
  - Is formed **between atoms that have similar** **electronegativities**.
  - Both atoms **have affinity for electrons** and **neither has a tendency to donate them**, they **share electrons** in order to achieve **octet configuration** and become **more stable**.

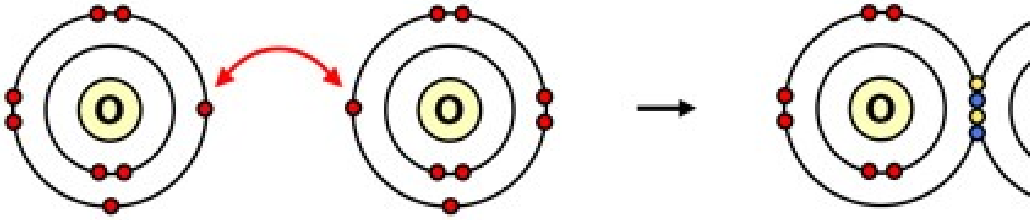


Covalent Bond Examples

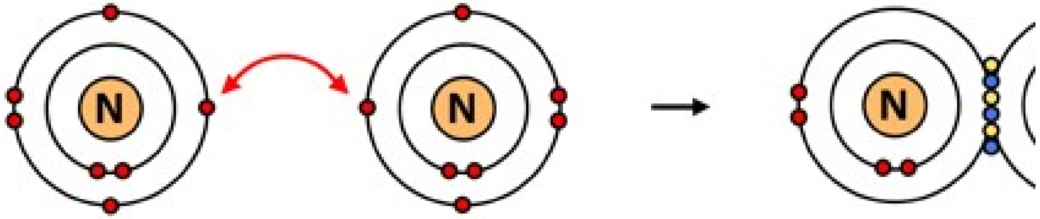
1. Chlorine (Cl_2)



2. Oxygen (O_2)



3. Nitrogen (N_2)



4. Hydrogen Chloride (HCl)

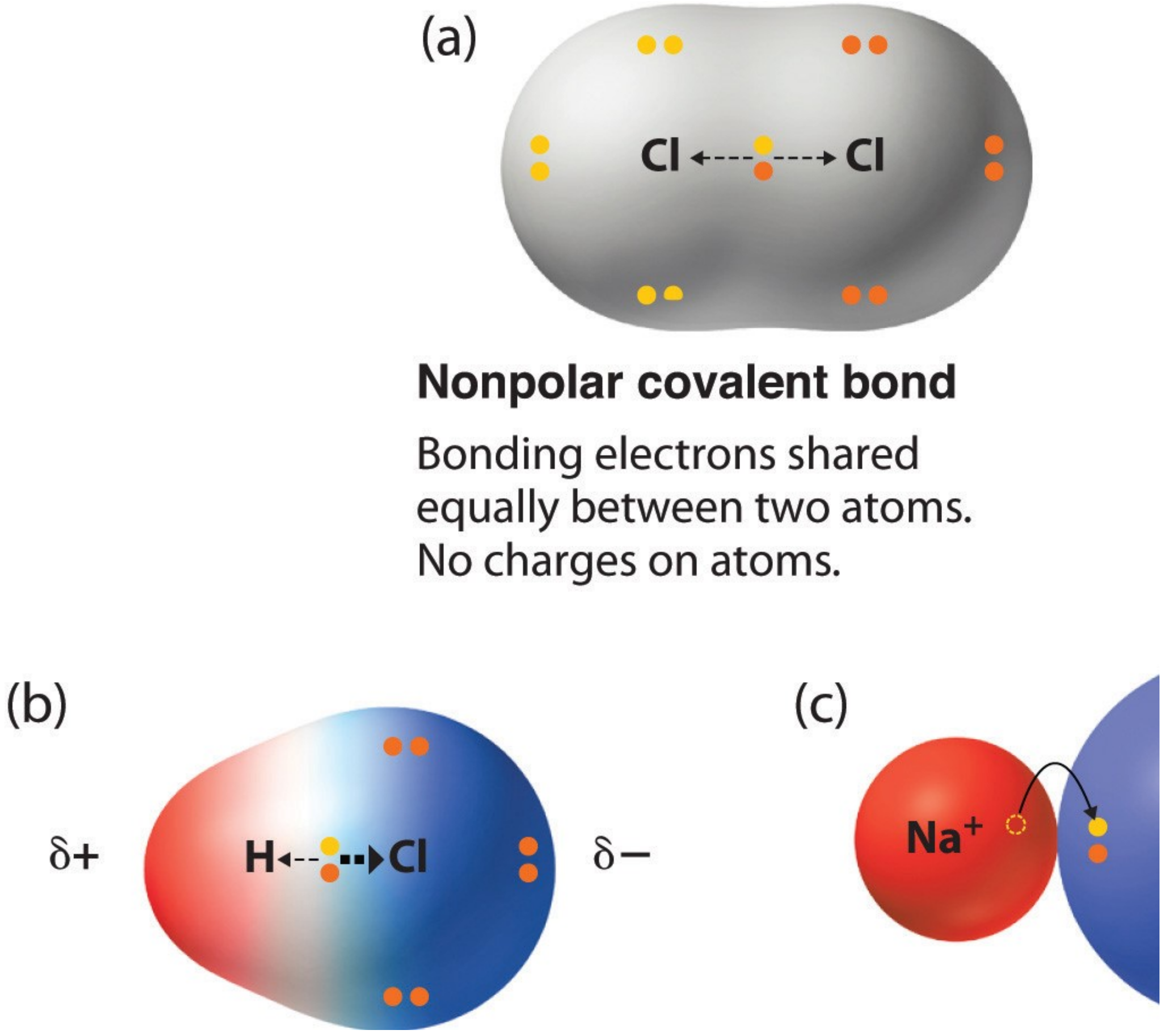
Periodic Table of the Elements

Atomic Number	Valence
Symbol	
Name	
Atomic Mass	

1 IA 1A	2 IIA 2A	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8	9 VIII 8	10	11 IB 1B	12 IIB 2B	13 IIIA 3A	14 IVA 4A	
1 -1, +1 **H** Hydrogen 1.008														
3 +1 **Li** Lithium 6.941	4 +2 **Be** Beryllium 9.012											5 +3 **B** Boron 10.811	6 +4,+3,+2,+1 -4,-3 -2,-1 **C** Carbon 12.011	7
11 +1 **Na** Sodium 22.990	12 +2 **Mg** Magnesium 24.305											13 +3 **Al** Aluminum 26.982	14 +4,-4 **Si** Silicon 28.086	15
19 +1 **K** Potassium 39.098	20 +2 **Ca** Calcium 40.078	21 +3 **Sc** Scandium 44.956	22 +4 **Ti** Titanium 47.88	23 +5 **V** Vanadium 50.942	24 +6,+3 **Cr** Chromium 51.996	25 +7,+4,+2 **Mn** Manganese 54.938	26 +6,+3,+2 **Fe** Iron 55.845	27 +3,+2 **Co** Cobalt 58.933	28 +2 **Ni** Nickel 58.693	29 +2 **Cu** Copper 63.546	30 +2 **Zn** Zinc 65.38	31 +3 **Ga** Gallium 69.723	32 +4,+2,-4 **Ge** Germanium 72.631	3
37 +1 **Rb** Rubidium 85.468	38 +2 **Sr** Strontium 87.62	39 +3 **Y** Yttrium 88.906	40 +4 **Zr** Zirconium 91.224	41 +5 **Nb** Niobium 92.906	42 +6,+4 **Mo** Molybdenum 95.95	43 +7,+4 **Tc** Technetium 98.907	44 +4,+3 **Ru** Ruthenium 101.07	45 +3 **Rh** Rhodium 102.906	46 +4,+2 **Pd** Palladium 106.42	47 +1 **Ag** Silver 107.868	48 +2 **Cd** Cadmium 112.414	49 +3 **In** Indium 114.818	50 +4,+2,-4 **Sn** Tin 118.711	5
55 +1 **Cs** Cesium 132.905	56 +2 **Ba** Barium 137.328	57-71	72 +4 **Hf** Hafnium 178.49	73 +5 **Ta** Tantalum 180.948	74 +6,+4 **W** Tungsten 183.85	75 +4 **Re** Rhenium 186.207	76 +4 **Os** Osmium 190.23	77 +4,+3 **Ir** Iridium 192.22	78 +4,+2 **Pt** Platinum 195.08	79 +3 **Au** Gold 196.967	80 +2,+1 **Hg** Mercury 200.59	81 +3,+1 **Tl** Thallium 204.383	82 +4,+2 **Pb** Lead 207.2	8
87 +1 **Fr** Francium 223.020	88 +2 **Ra** Radium 226.025	89-103	104 +4 **Rf** Rutherfordium [261]	105 +5 **Db** Dubnium [262]	106 +6 **Sg** Seaborgium [266]	107 +7 **Bh** Bohrium [264]	108 +8 **Hs** Hassium [269]	109 unknown **Mt** Meitnerium [278]	110 unknown **Ds** Darmstadtium [281]	111 unknown **Rg** Roentgenium [280]	112 +2 **Cn** Copernicium [285]	113 unknown **Nh** Nihonium [286]	114 unknown **Fl** Flerovium [289]	11

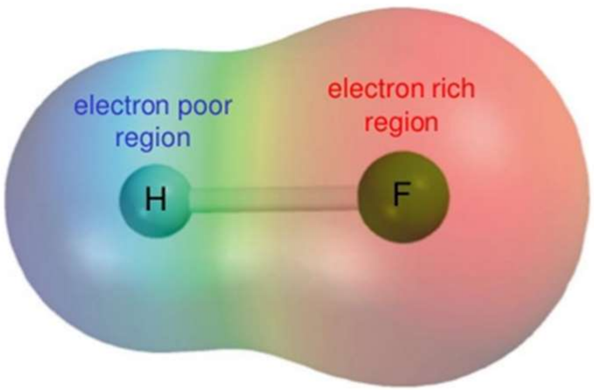
Lanthanide Series	57 +3 **La** Lanthanum 138.905	58 +4,+3 **Ce** Cerium 140.116	59 +3 **Pr** Praseodymium 140.908	60 +3 **Nd** Neodymium 144.243	61 +3 **Pm** Promethium 144.913	62 +3 **Sm** Samarium 150.36	63 +3,+2 **Eu** Europium 151.964	64 +3 **Gd** Gadolinium 157.25	65 +3 **Tb** Terbium 158.925	66 +3 **Dy** Dysprosium 162.500	67 +3 **Ho** Holmium 164.930	68 **Er** Erbium 167.25
Actinide	89 +3 **Ac**	90 +4 **Th**	91 +5 **Pa**	92 +6 **U**	93 +5 **Np**	94 +4 **Pu**	95 +3 **Am**	96 +3 **Cm**	97 +3 **Bk**	98 +3 **Cf**	99 +3 **Es**	100 **Fm**

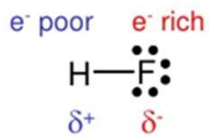
Covalent or Ionic bondings depend on …

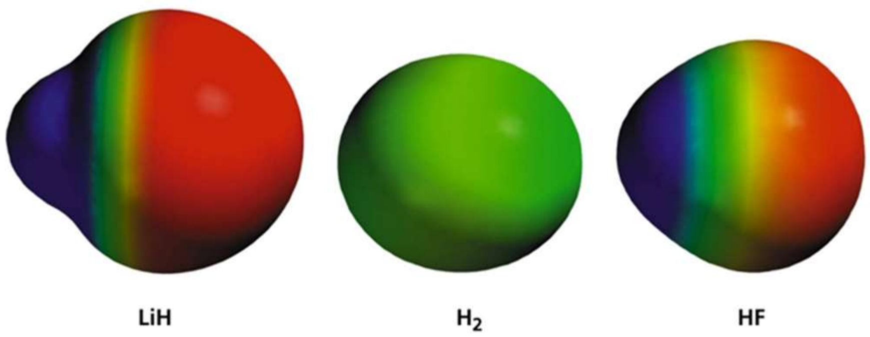


Electron Density

- **Polar covalent bond** is a covalent bond with **greater electron density** around **one of the two atoms.**
- Electron cloud **moves towards the atoms that have higher masses** or **more electronegative**.
- Eg… HF (Hydrogen flouride; H – F bond)

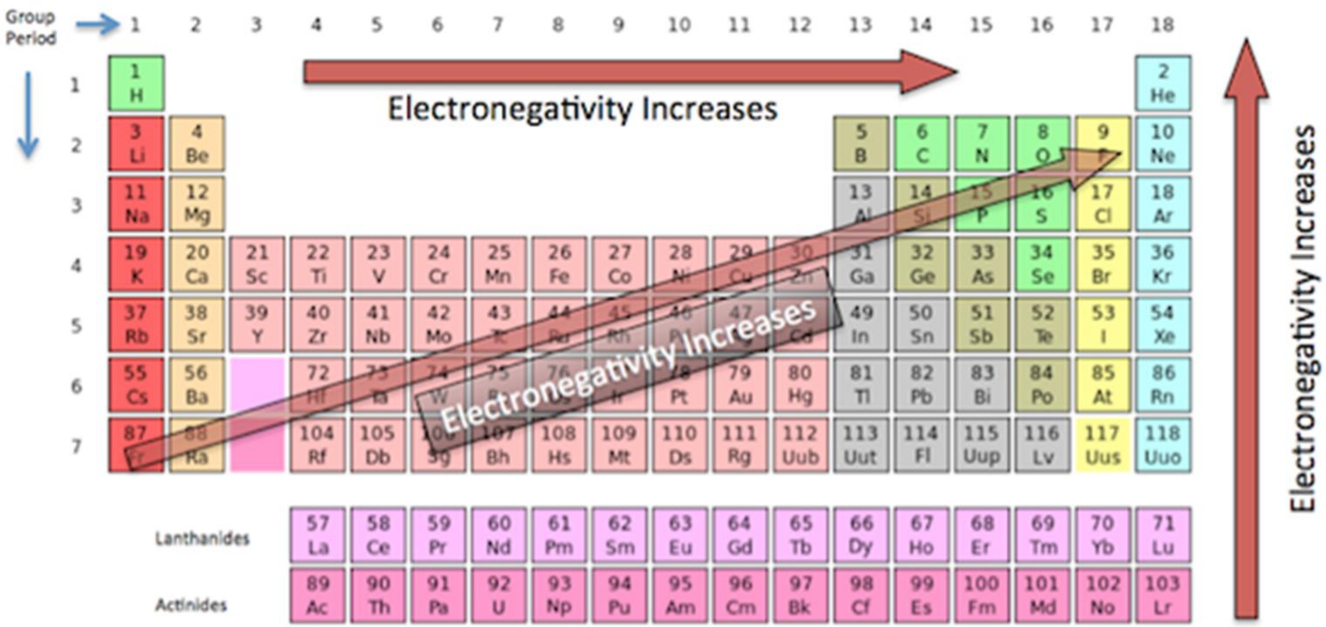






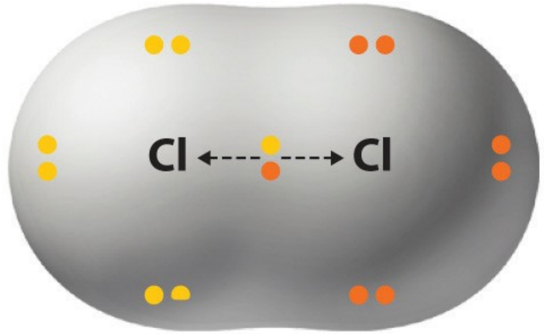
Electronegativity

- Is the **ability or power** of an atom in a molecule to **attract electrons to itself in a chemical bonding** **(described by Linus Pauling).**
  - Basically, is a **relative value** of that **atom's ability to attract electron density toward itself when it bonds to another atom.**
  - **The higher the electronegative of an element → the more that atom pick up electron easily.**



Electronegativity Trend

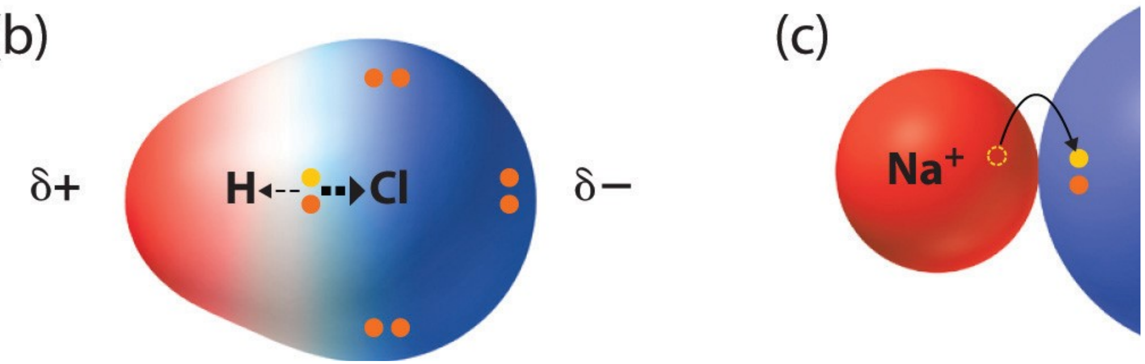
(a)



Nonpolar covalent bond

Bonding electrons shared equally between two atoms. No charges on atoms.

(b) (c)



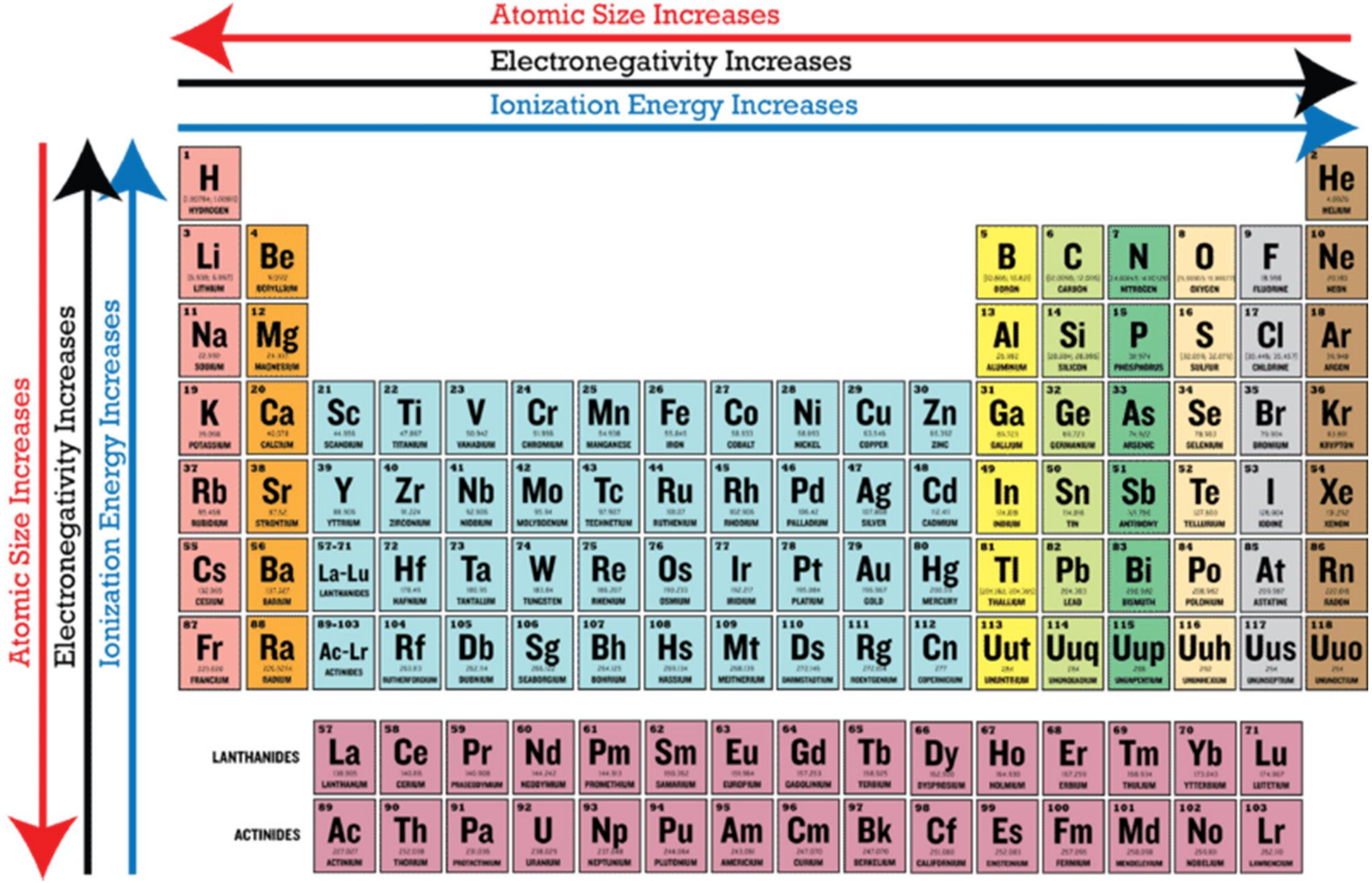
Automic radius decreases → Ionization energy increases → Electronegativity increases

Pauling Scale

0.7 – 3.98

Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H 2.20																	He
2	Li 0.98	Be 1.57											B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne
3	Na 0.93	Mg 1.31											Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar
4	K 0.82	Ca 1.00	Sc 1.36	Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 1.90	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr
5	Rb 0.82	Sr 0.95	Y 1.22	Zr 1.33	Nb 1.6	Mo 2.16	Tc 2.10	Ru 2.2	Rh 2.28	Pd 2.20	Ag 1.93	Cd 1.69	In 1.78	Sn 1.96	Sb 2.05	Te 2.1	I 2.66	Xe
6	Cs 0.79	Ba 0.89	La 1.10	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	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2	Rn
7	Fr 0.7	Ra 0.9	Ac 1.1	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Uub	Uut	Uuq	Uup			

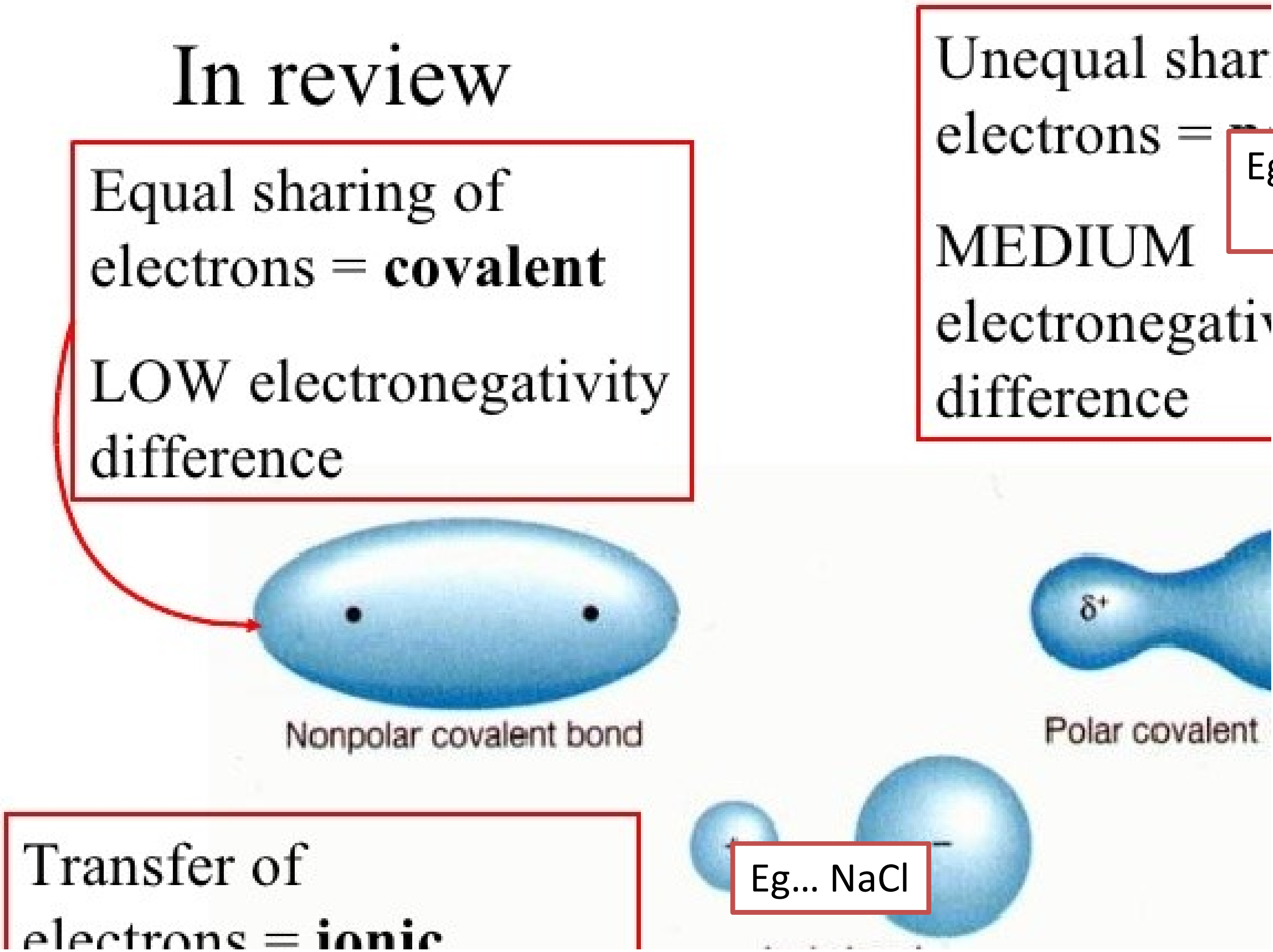
Lanthanides 6	Ce 1.12	Pr 1.13	Nd 1.14	Pm	Sm 1.17	Eu	Gd 1.20	Tb	Dy 1.22	Ho 1.23	Er 1.24	Tm 1.25	Yb	Lu 1.0
Actinides 7	Th 1.3	Pa 1.5	U 1.7	Np 1.3	Pu 1.3	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr



Atomic Size Increases
Electronegativity Increases
Ionization Energy Increases
Atomic Size Increases
Electronegativity Increases
Ionization Energy Increases
1 H
2 He
3 Li
4 Be
5 B
6 C
7 N
8 O
9 F
10 Ne
11 Na
12 Mg
13 Al
14 Si
15 P
16 S
17 Cl
18 Ar
19 K
20 Ca
21 Sc
22 Ti
23 V
24 Cr
25 Mn
26 Fe
27 Co
28 Ni
29 Cu
30 Zn
31 Ga
32 Ge
33 As
34 Se
35 Br
36 Kr
37 Rb
38 Sr
39 Y
40 Zr
41 Nb
42 Mo
43 Tc
44 Ru
45 Rh
46 Pd
47 Ag
48 Cd
49 In
50 Sn
51 Sb
52 Te
53 I
54 Xe
55 Cs
56 Ba
57-71 La-Lu
72 Hf
73 Ta
74 W
75 Re
76 Os
77 Ir
78 Pt
79 Au
80 Hg
81 Tl
82 Pb
83 Bi
84 Po
85 At
86 Rn
87 Fr
88 Ra
89-103 Ac-Lr
104 Rf
105 Db
106 Sg
107 Bh
108 Hs
109 Mt
110 Ds
111 Rg
112 Cn
113 Uut
114 Uuq
115 Uup
116 Uuh
117 Uus
118 Uuo
LANTHANIDES
57 La
58 Ce
59 Pr
60 Nd
61 Pm
62 Sm
63 Eu
64 Gd
65 Tb
66 Dy
67 Ho
68 Er
69 Tm
70 Yb
71 Lu
ACTINIDES
89 Ac
90 Th
91 Pa
92 U
93 Np
94 Pu
95 Am
96 Cm
97 Bk
98 Cf
99 Es
100 Fm
101 Md
102 No
103 Lr

What if two atoms of equal or more electronegativity bond together?

Eg… H_2 or Cl_2



Eg… H_2O or HCl

Eg… NaCl

Electronegativity (EN)

V · T · E

Periodic table of electronegativity by Pauling scale

→ Atomic radius decreases → Ionization energy increases → Electronegativity increases →

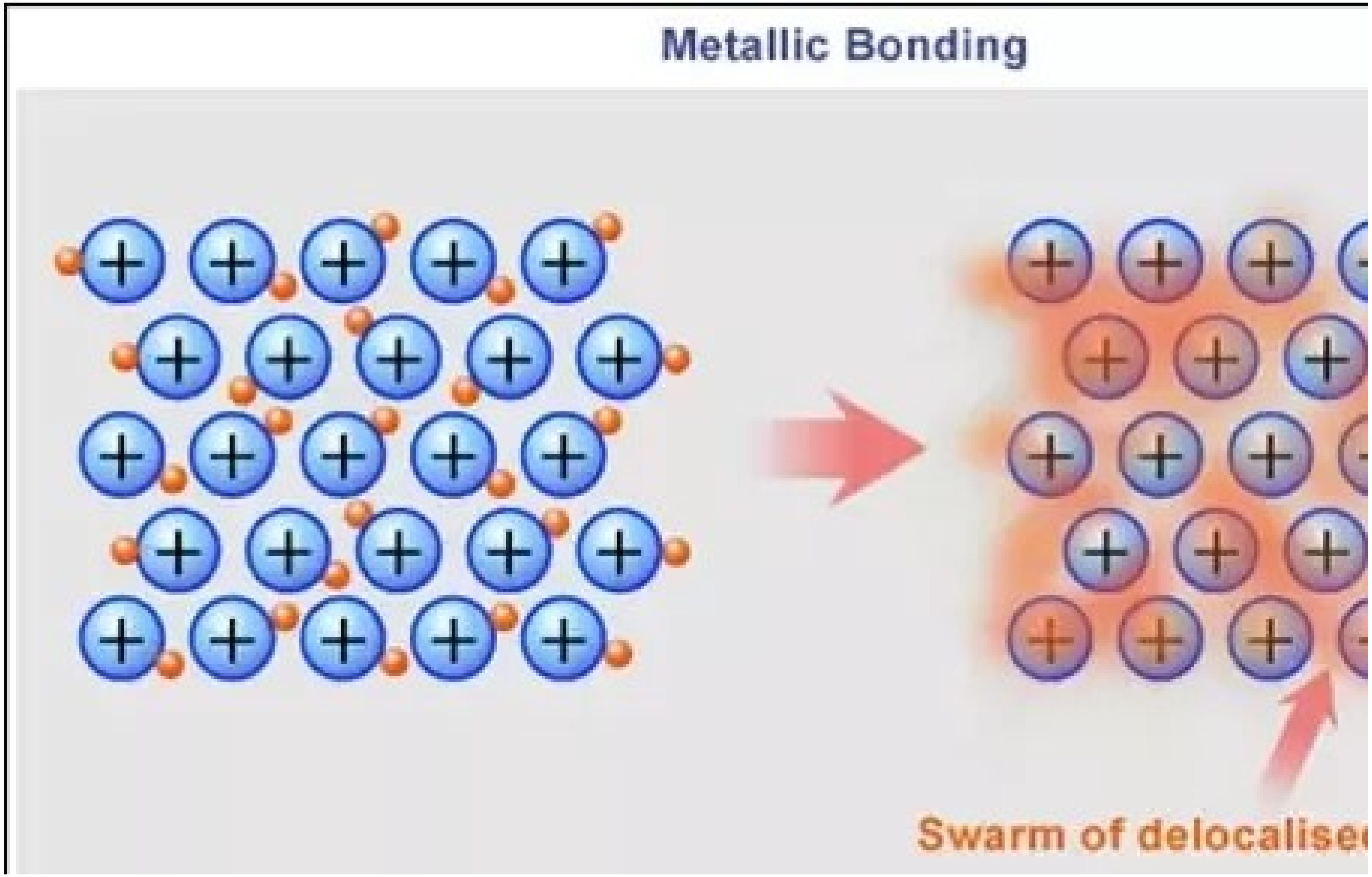
Group → / ↓ Period	1	2	3		4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H 2.20																		He
2	Li 0.98	Be 1.57												B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne
3	Na 0.93	Mg 1.31												Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar
4	K 0.82	Ca 1.00	Sc 1.36		Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 1.90	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr 3.00
5	Rb 0.82	Sr 0.95	Y 1.22		Zr 1.33	Nb 1.6	Mo 2.16	Tc 1.9	Ru 2.2	Rh 2.28	Pd 2.20	Ag 1.93	Cd 1.69	In 1.78	Sn 1.96	Sb 2.05	Te 2.1	I 2.66	Xe 2.60
6	Cs 0.79	Ba 0.89	La 1.1	*	Hf 1.3	Ta 1.5	W 2.36	Re 1.9	Os 2.2	Ir 2.20	Pt 2.28	Au 2.54	Hg 2.00	Tl 1.62	Pb 1.87	Bi 2.02	Po 2.0	At 2.2	Rn 2.2
7	Fr 0.7[en 1]	Ra 0.9	Ac 1.1	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og

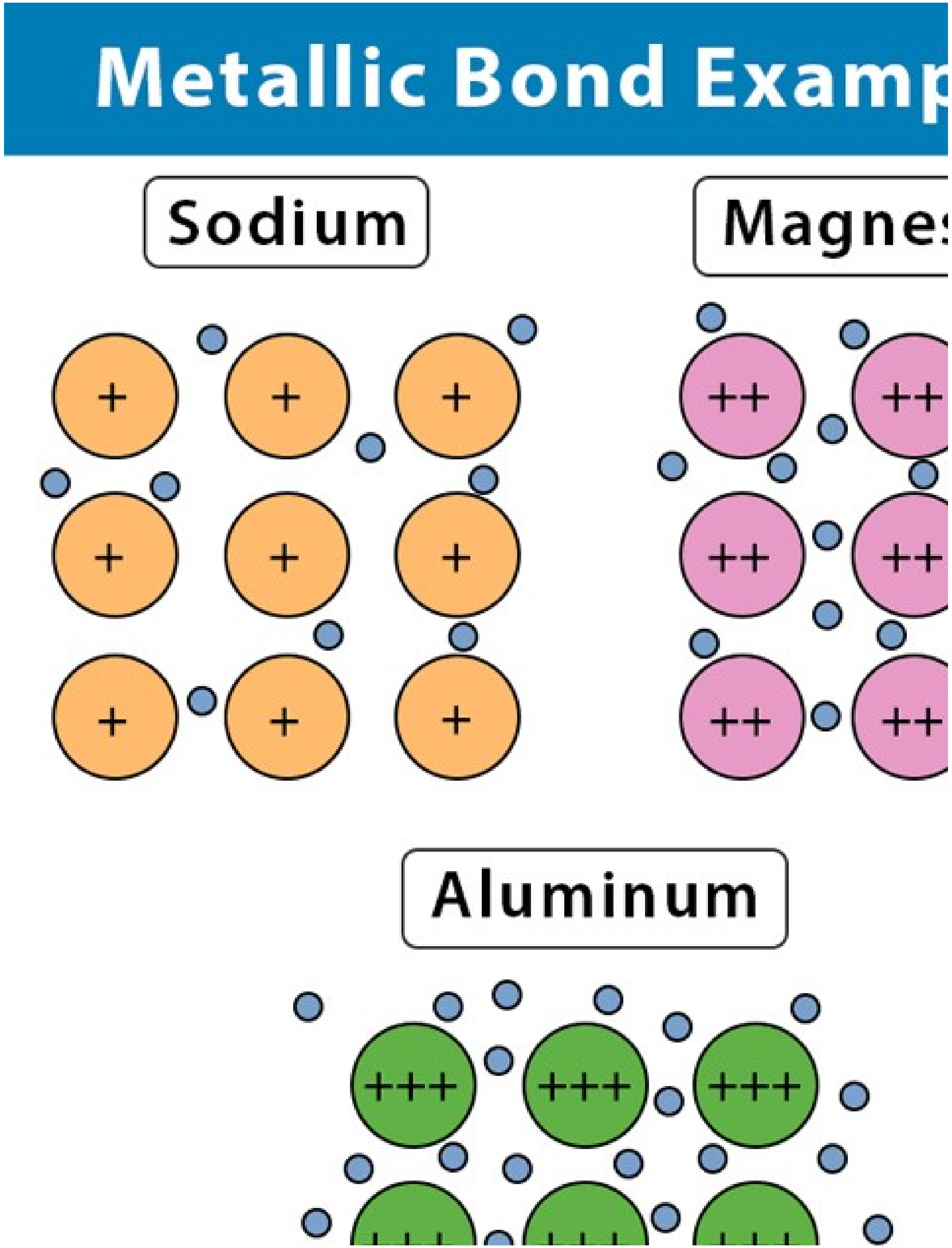
*	Ce 1.12	Pr 1.13	Nd 1.14	Pm 1.13	Sm 1.17	Eu 1.2	Gd 1.2	Tb 1.1	Dy 1.22	Ho 1.23	Er 1.24	Tm 1.25	Yb 1.1	Lu 1.27
**	Th 1.3	Pa 1.5	U 1.38	Np 1.36	Pu 1.28	Am 1.13	Cm 1.28	Bk 1.3	Cf 1.3	Es 1.3	Fm 1.3	Md 1.3	No 1.3	Lr 1.3[en 2]

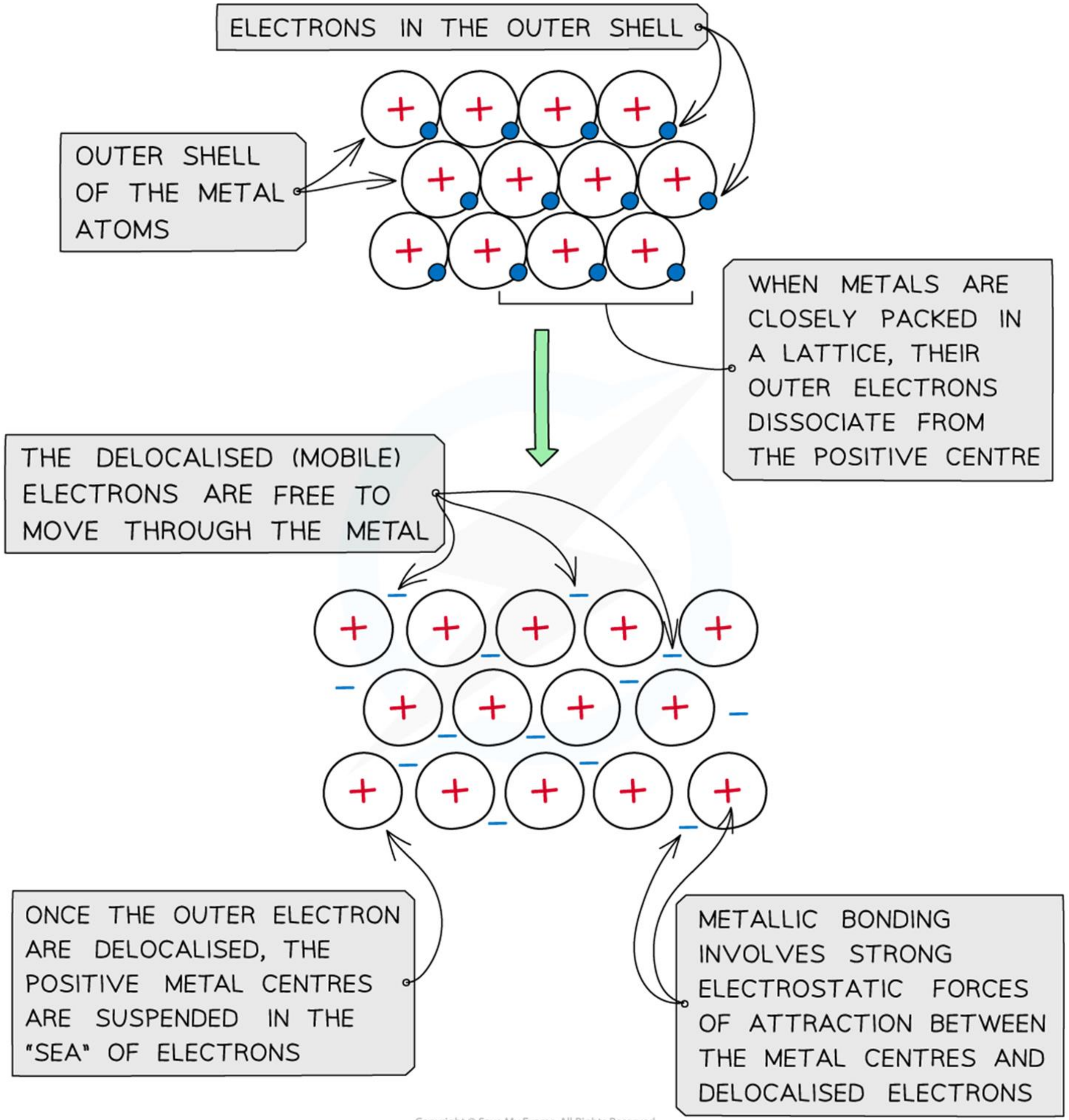
Values are given for the elements in their most common and stable oxidation states.

See also: Electronegativities of the elements (data page)

Metallic Bonding




Metallic Bond Examp
Sodium
Magnes
Aluminum
+
++
+++


ELECTRONS IN THE OUTER SHELL
OUTER SHELL OF THE METAL ATOMS
WHEN METALS ARE CLOSELY PACKED IN A LATTICE, THEIR OUTER ELECTRONS DISSOCIATE FROM THE POSITIVE CENTRE
THE DELOCALISED (MOBILE) ELECTRONS ARE FREE TO MOVE THROUGH THE METAL
ONCE THE OUTER ELECTRON ARE DELOCALISED, THE POSITIVE METAL CENTRES ARE SUSPENDED IN THE "SEA" OF ELECTRONS
METALLIC BONDING INVOLVES STRONG ELECTROSTATIC FORCES OF ATTRACTION BETWEEN THE METAL CENTRES AND DELOCALISED ELECTRONS

Metallic Bonding

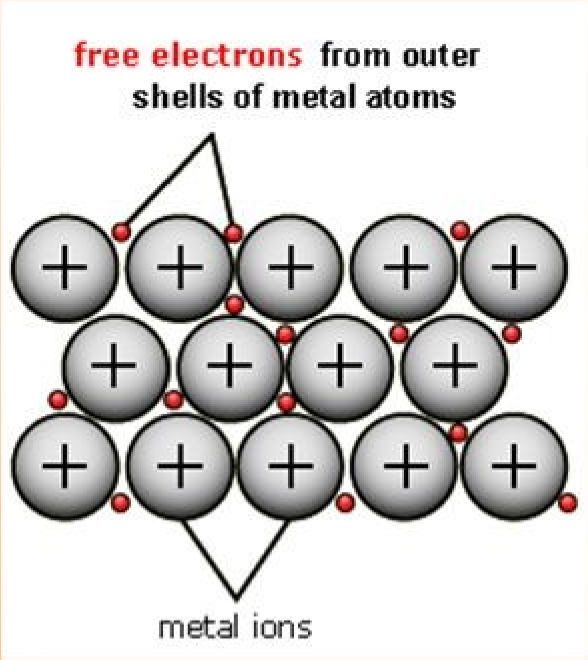
Most elements are metals:

- Hard
- Shiny
- Good **conductors** of heat and electricity
- High **tensile strength** (resist stretching)
- High melting and boiling points (strong bonds)

Positive metal ions closely together

Sea of free (delocalised) electrons

Strong attraction between metal ions and electrons = Very strong bonds



Comparing and Contrasting Ionic, Covalent a Bonds

	Ionic Bonds	Covalent Bonds	M
Electrons	Transferred	Shared, evenly or unevenly	
Bond	Metal to Nonmetal	Nonmetal to Nonmetal	M
Electronegativity Differences	Differences **greater than 2.0**	Differences **betwn 0.0 and 2.0**	
Make Compounds	Yes, by attraction of opposite charged ions	Molecules, or molecular elements	
State (STP)	Crystalline solid	Liquid, gas, or solid	N
rties Melting Pt	high	low	

N/A: Not Applicable or No Answer

Pauling Scale

0.7 3.98

Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H 2.20																	He
2	Li 0.98	Be 1.57											B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne
3	Na 0.93	Mg 1.31											Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar
4	K 0.82	Ca 1.00	Sc 1.36	Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 1.90	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr
5	Rb 0.82	Sr 0.95	Y 1.22	Zr 1.33	Nb 1.6	Mo 2.16	Tc 2.10	Ru 2.2	Rh 2.28	Pd 2.20	Ag 1.93	Cd 1.69	In 1.78	Sn 1.96	Sb 2.05	Te 2.1	I 2.66	Xe
6	Cs 0.79	Ba 0.89	La 1.10	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	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2	Rn
7	Fr 0.7	Ra 0.9	Ac 1.1	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Uub	Uut	Uuq	Uup			

Lanthanides 6	Ce 1.12	Pr 1.13	Nd 1.14	Pm	Sm 1.17	Eu	Gd 1.20	Tb	Dy 1.22	Ho 1.23	Er 1.24	Tm 1.25	Yb	Lu 1.0
Actinides 7	Th 1.3	Pa 1.5	U 1.7	Np 1.3	Pu 1.3	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Intermolecular Forces

are attractive forces b/t molecules

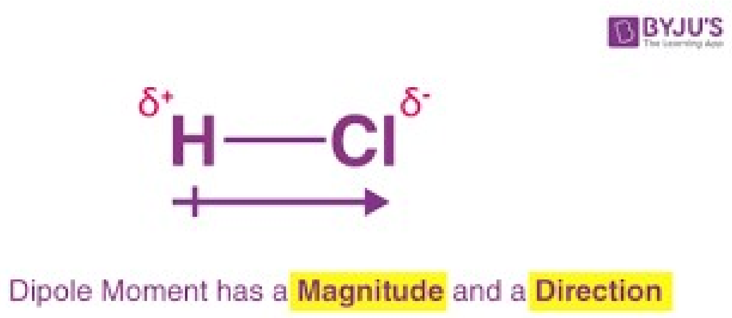
- Dipole – Dipole Interactions
- Hydrogen Bonding
- Van Der Waals Forces

<u>Intermolecular vs Intramolecular</u>

- 41 kJ to vaporize 1 mole of water (**inter**)
- 930 kJ to break all O-H bonds in 1 mole of water (**intra**)

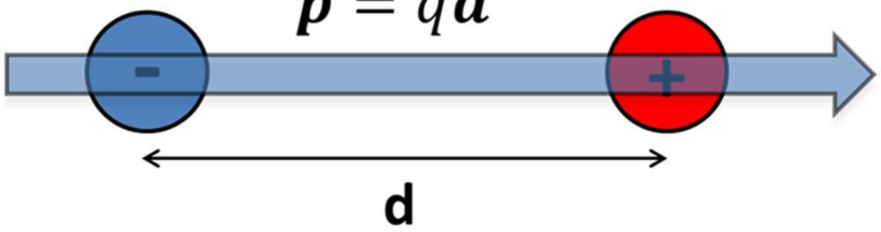
Dipole & Dipole Moment

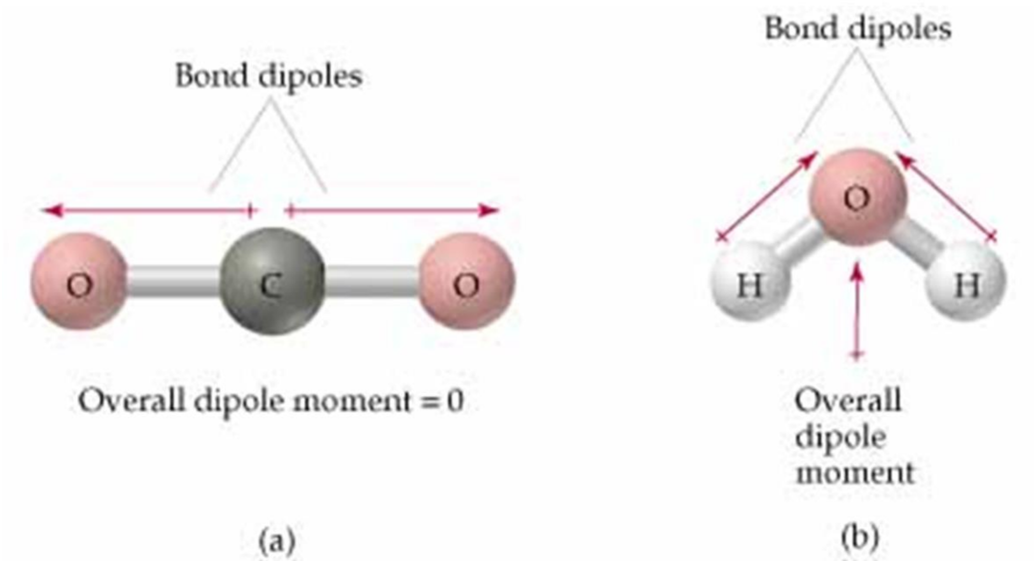
- **Dipole** occur when there is a **separation of charge**.
- **Dipole moment** is a measure of the **polarity of the molecule**.
  - Can occur between **two ions in an ionic bond** or **between atoms in a covalent bond**.
  - **Arise from differences in electronegativity**.
  - The **larger** the **difference in electronegativity**, the **greater** the **dipole moment**.
  - The size of the dipole moment also depends on the distance between the charge separation.

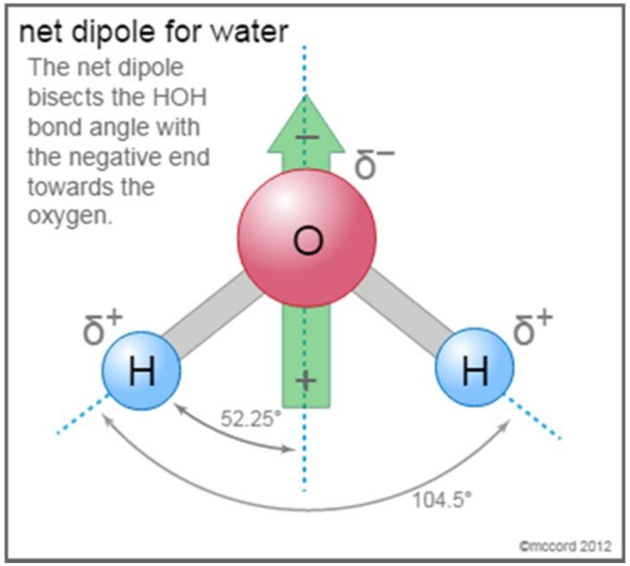


Dipole & Dipole Moment

$$\vec{p} = q\vec{d}$$

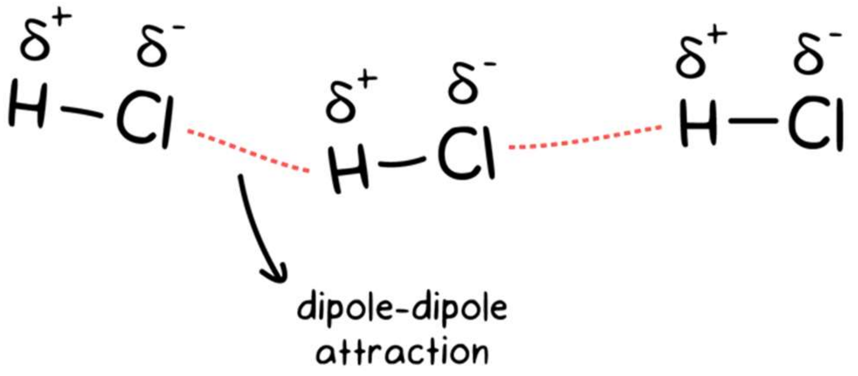


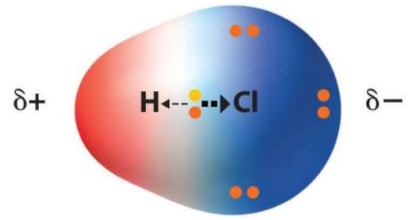




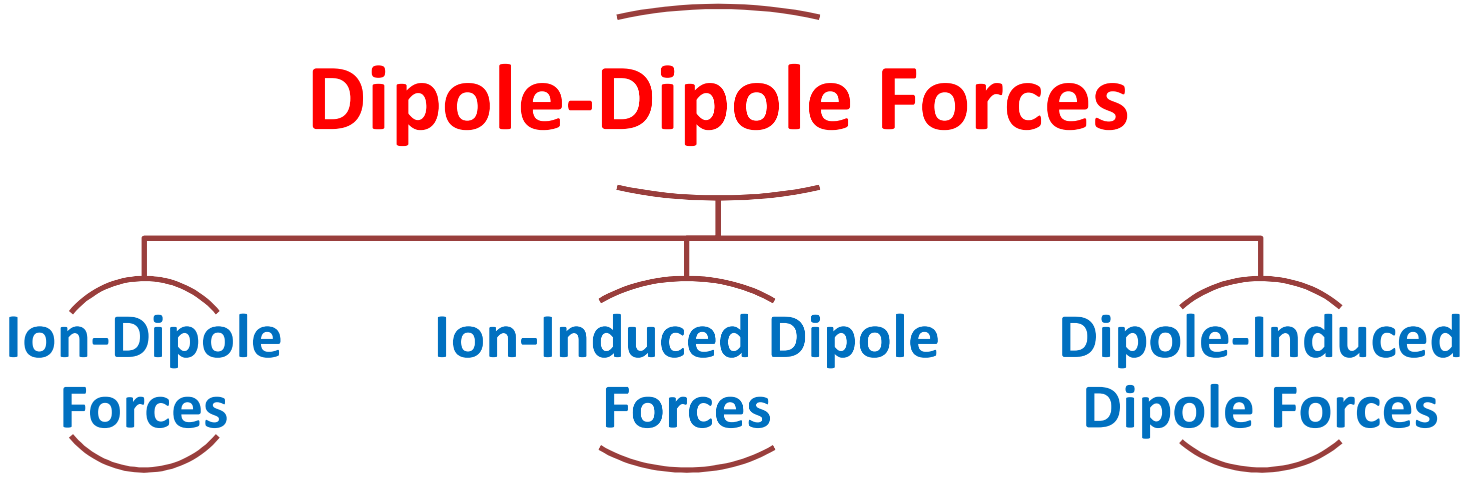
Intermolecular Forces

- **Dipole – Dipole Forces (Interactions)**
  - **Are the attractive forces b/t polar molecules.**
  - Occur when the **partially positively charged part of a molecule** interacts with the **partially negatively charged part of the neighboring molecule**.
  - **The prerequisite for this type of attraction to exist is partially charged ions, Eg…** HCl.
  - ***Are the strongest intermolecular force of attraction, after hydrogen bonds***.



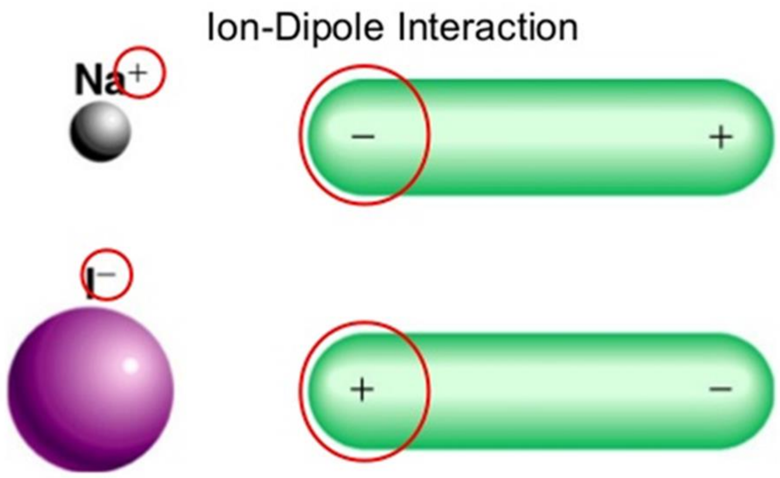


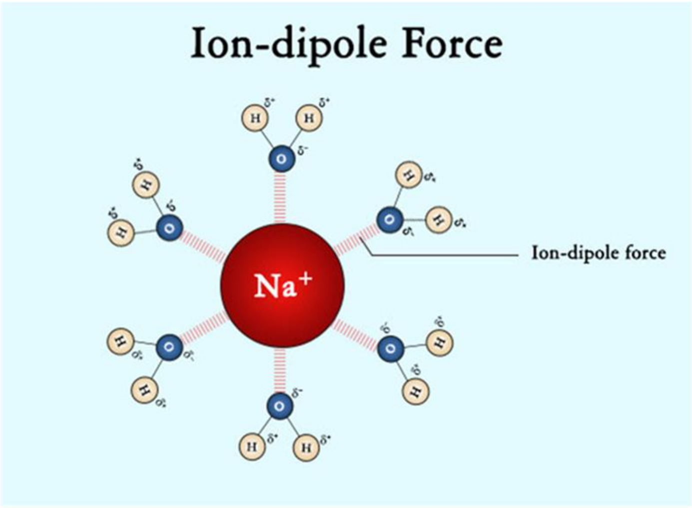
$$U_{dipol-dipol} = -\frac{2\mu'^2\mu^2}{3kTr^6}$$


Dipole-Dipole Forces
Ion-Dipole Forces
Ion-Induced Dipole Forces
Dipole-Induced Dipole Forces

Ion-Dipole Forces

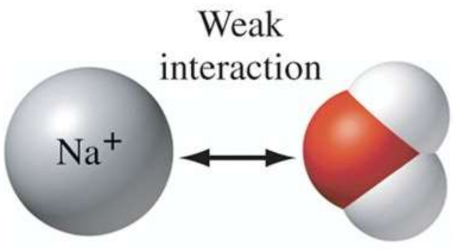
Attractive forces between an **ion** and a **polar molecule**

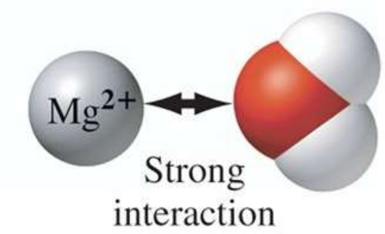


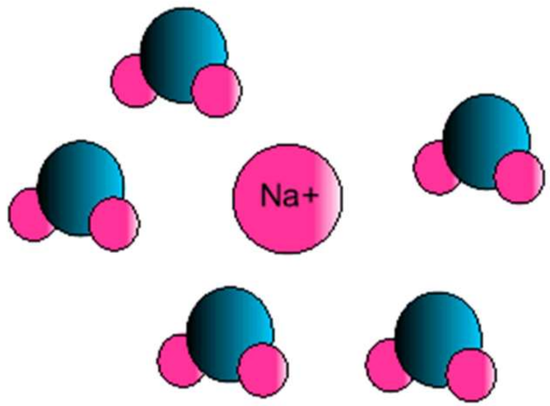


When NaCl is dissolved in water, it will dissociate into Na+ ions and Cl- ions; the force of attraction that may exist between, say, Na+ and the -δ oxygen of water is nothing but ion-dipole force. It is due to this force of attraction that the polar molecule will dissolve in a polar solvent like water.

Ion-dipole interactions are Coulombic attractions between ions (either positive or negative) and polar molecules.

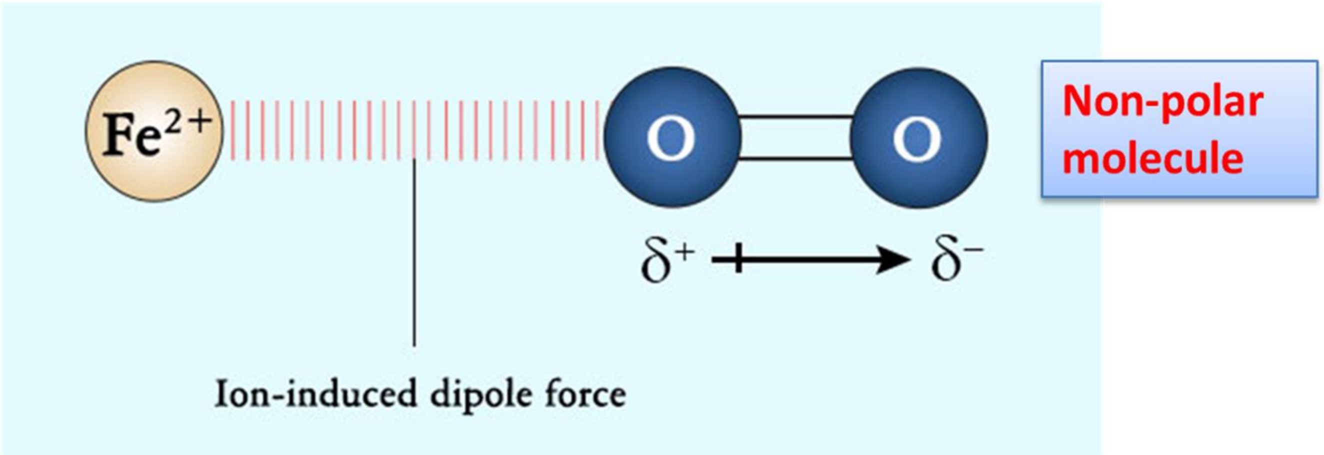






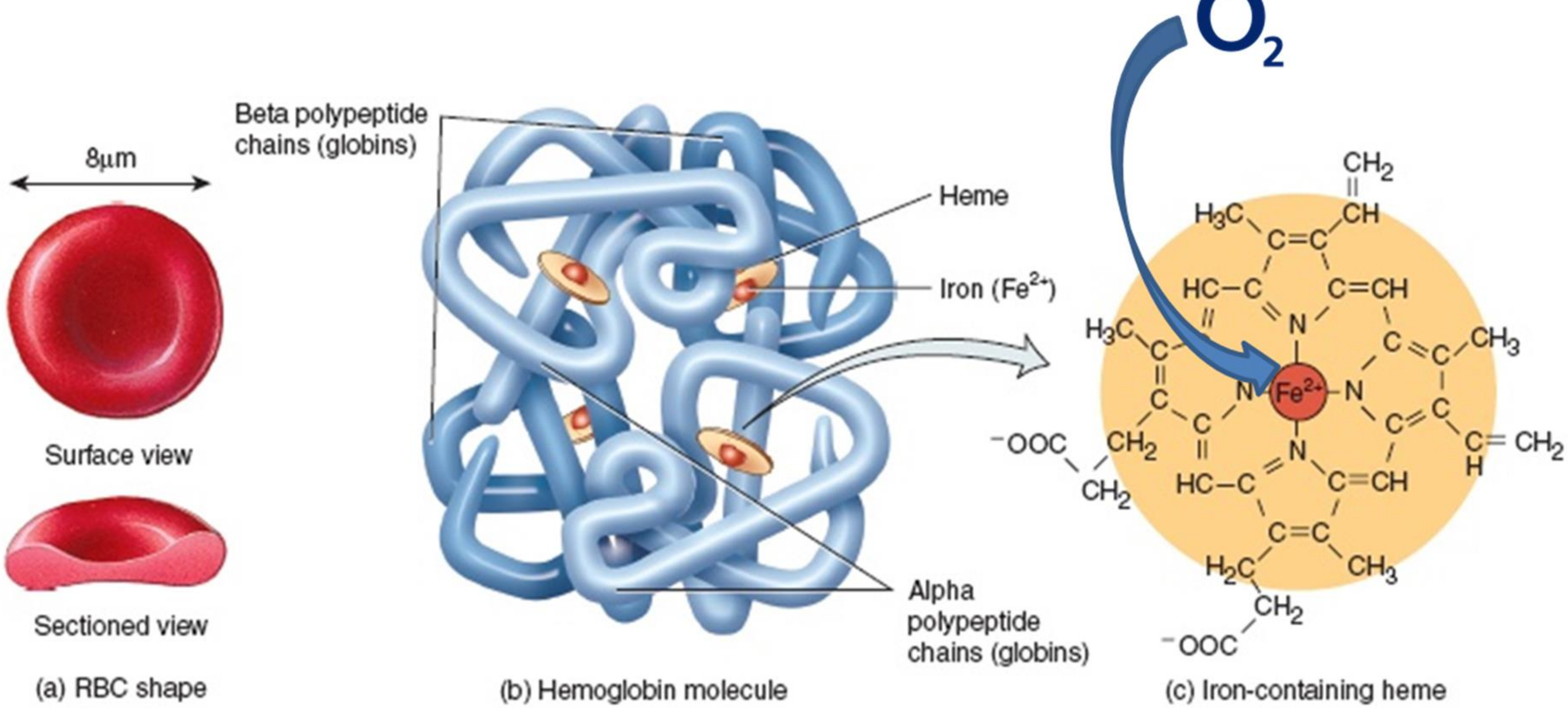
Ion-induced Dipole Forces

Occurs when an ion interacts with a non-polar molecule.

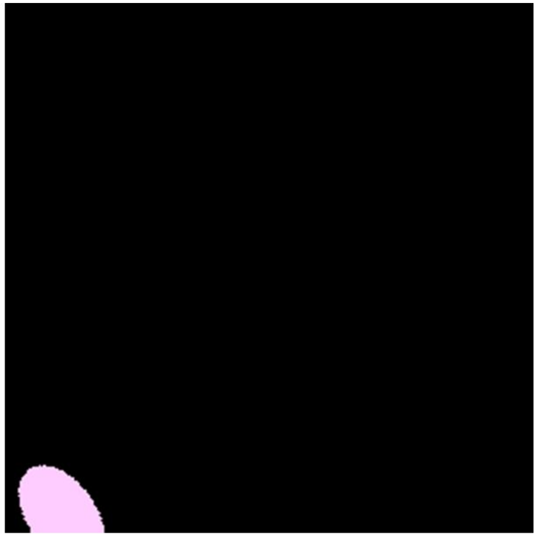


In this, the ion may attract or repel the electron cloud present on the non-polar molecule and induce the non-polar molecule to become a temporary dipole. The strength of this induced dipole depends on how easily the electron cloud can be distorted, i.e., the bigger the molecule, the stronger is the dipole induced.

Hemoglobin

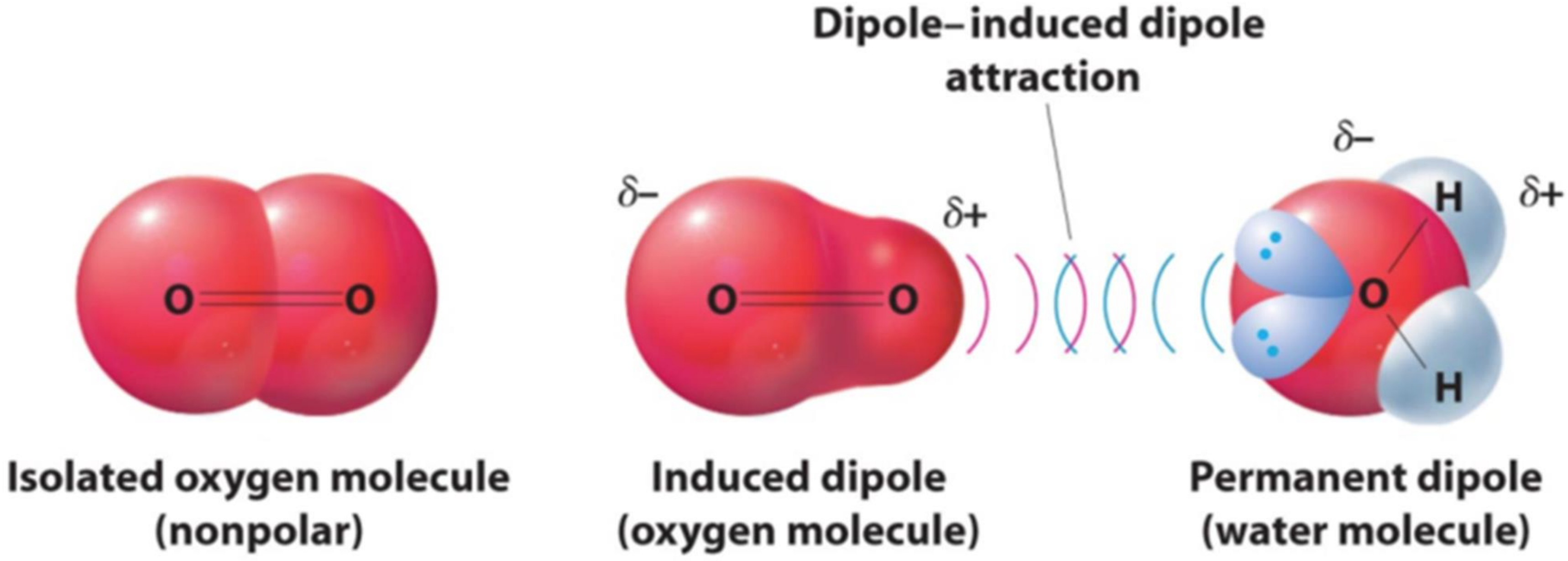


Fe^{2+} ion attracts the O_2 by ion-induced dipole force.



Dipole-induced Dipol Forces

Occur when a non-polar molecule interacts with a polar molecule.



A non-polar molecule turns into a induced dipole when it interacts with a polar molecule.

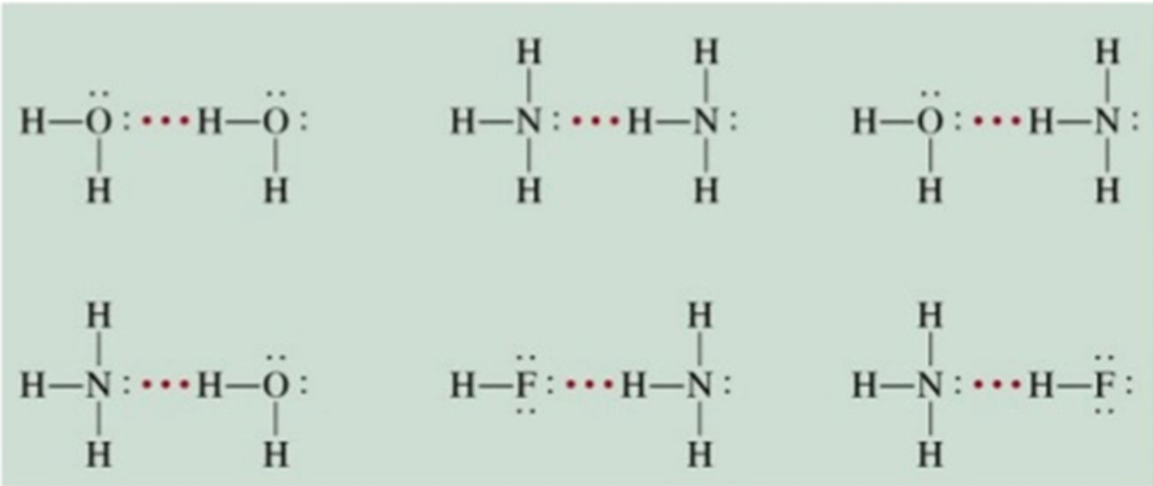
Intermolecular Forces

Hydrogen Bond

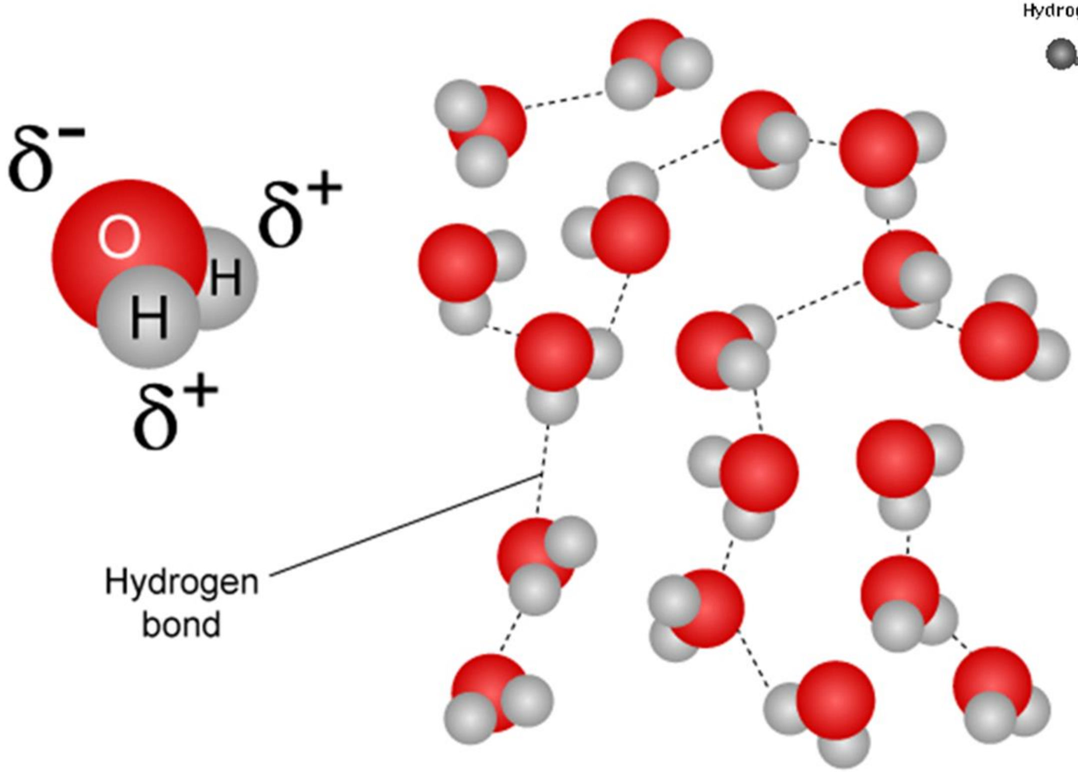
The ***hydrogen bond*** is a special dipole-dipole interaction between the hydrogen atom in a polar N-H, O-H, or F-H bond and an electronegative O, N, or F atom.

$$A - H \cdots B \quad \text{or} \quad A - H \cdots A$$

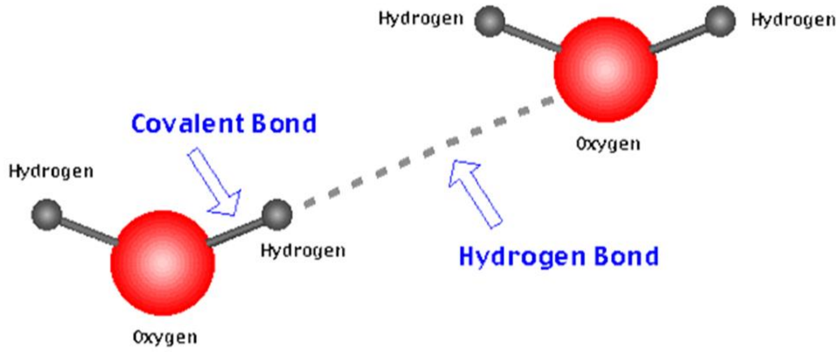
A & B are N, O, or F



Hydrogen Bond Energy: 4 – 29 kJ/mol (0.25 – 7.25 kcal/mol).

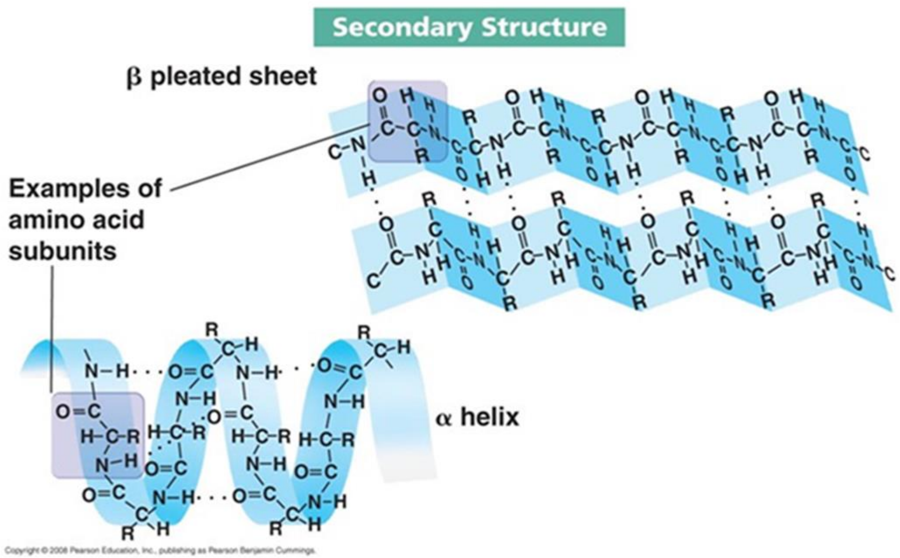


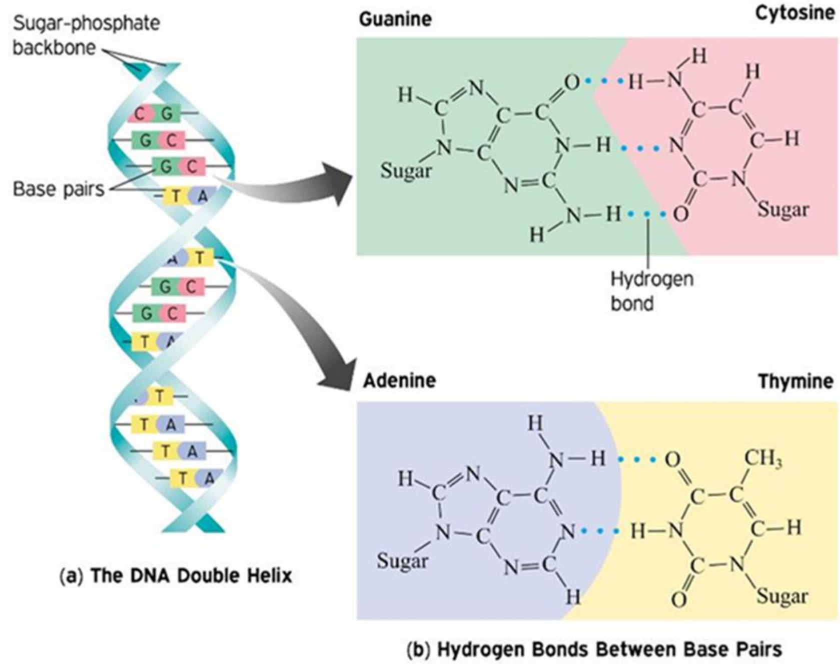
(length appears different for perspective (3D))



The partially positive end of hydrogen is attracted to the partially negative end of the oxygen molecule.

H-bond in Proteins & Nucleic Acids





Intermolecular Forces

Van der Waals (VDW) Forces

❑ Its main characteristics are:-

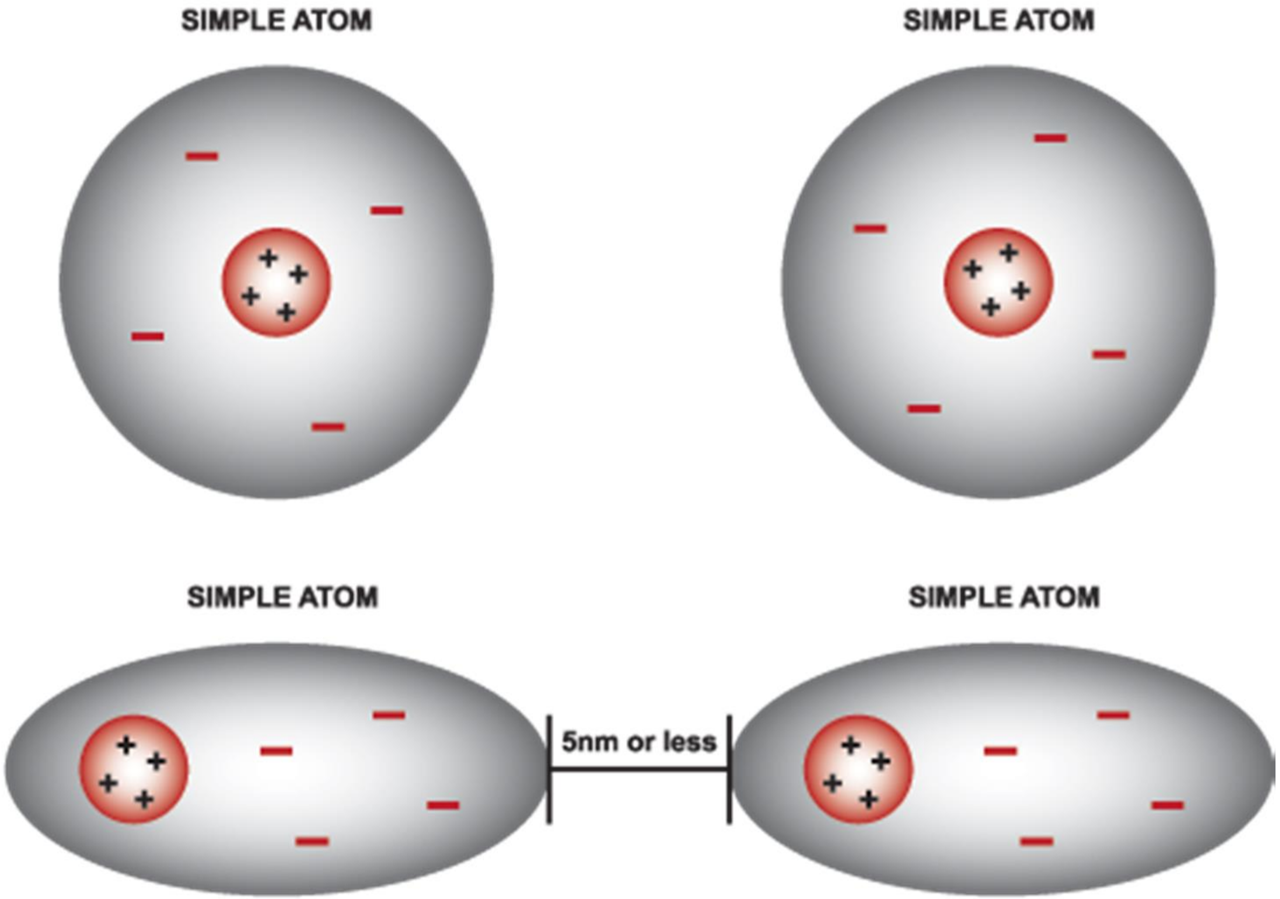
- They are weaker than normal covalent ionic bonds.
- Van der Waals forces are additive and cannot be saturated.
- They have no directional characteristic.
- They are all short - range forces and hence only interactions between nearest need to be considered instead of all the particles. The greater is the attraction if the molecules are closer due to Van der Waals forces.
- Van der Waals forces are independent of temperature

VAN DER WAALS' FORCES (VDW) DIAGRAM

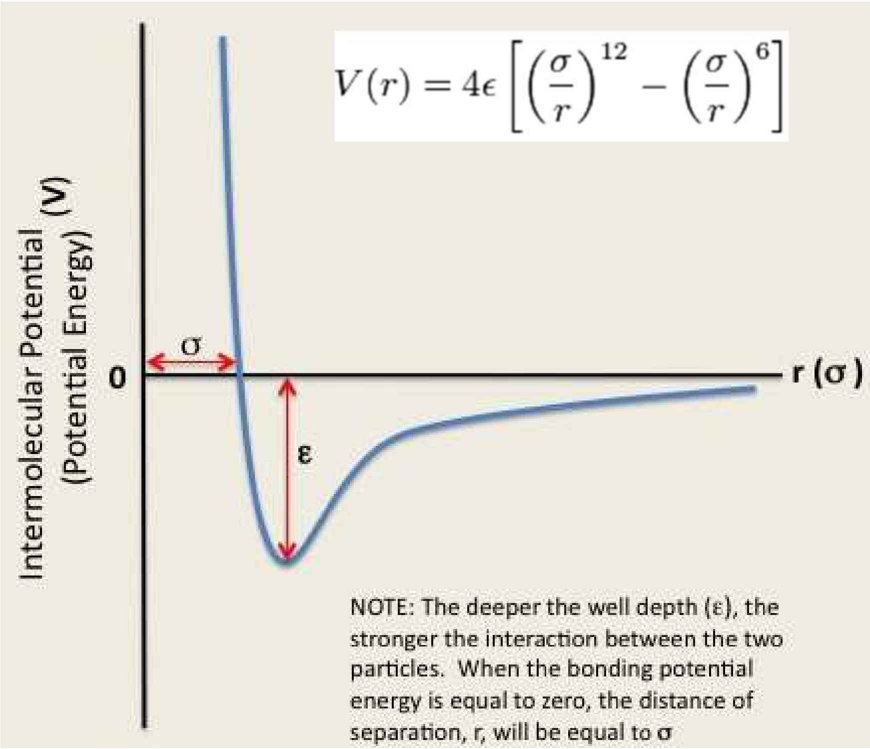
KEY

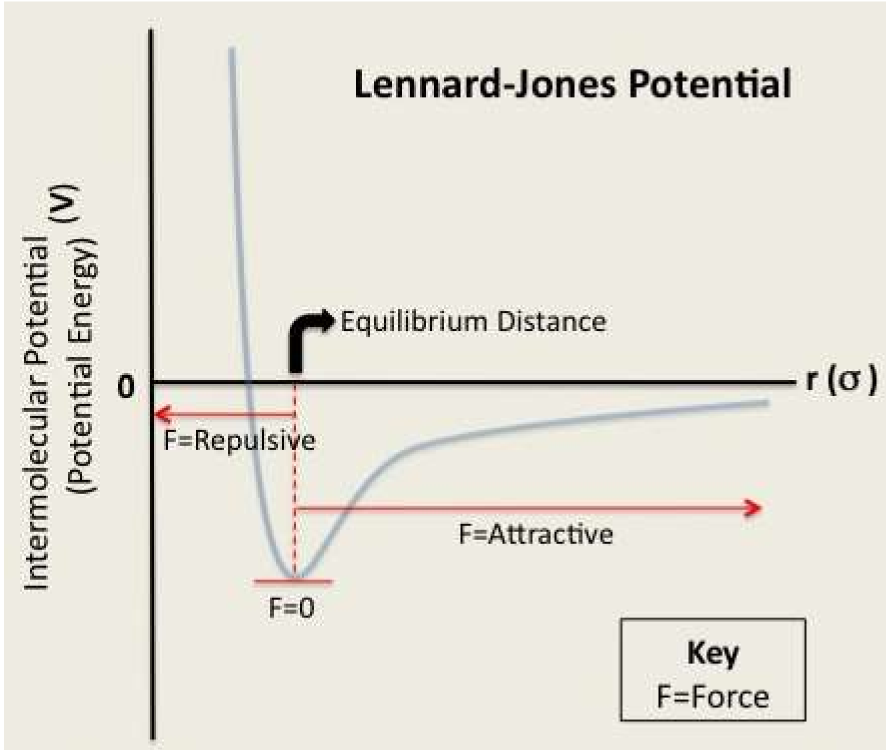
+ POSITIVE NUCLEUS

— NEGATIVE CHARGED ELECTRON CLOUD



When two atoms come within 5 nanometers of each other, there will be a slight interaction between them, thus causing polarity and a slight attraction.





- **σ** gives a measurement of **how close two non-bonding particles can get** and is **thus referred to as** the *van der Waals radius*.

- It is equal to one-half of the internuclear distance between non-bonding particles.

Van Der Waals (VDW) Forces

VDW Forces
are weak polar interactions

Keesom Interaction

weak dipole – dipole interaction

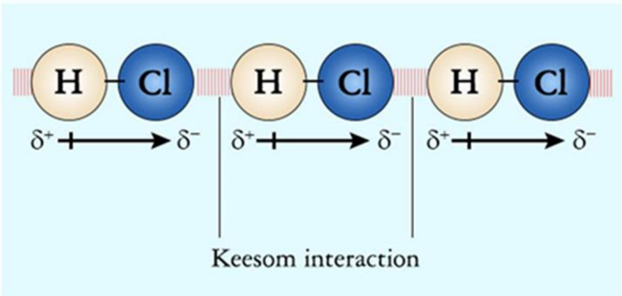
Debye Interaction

weak dipole – induced dipole interaction

London Dispertion Forces

instantaneous induced dipole

VDW Forces: Keesom Interaction (Force btw two permanent dipoles)



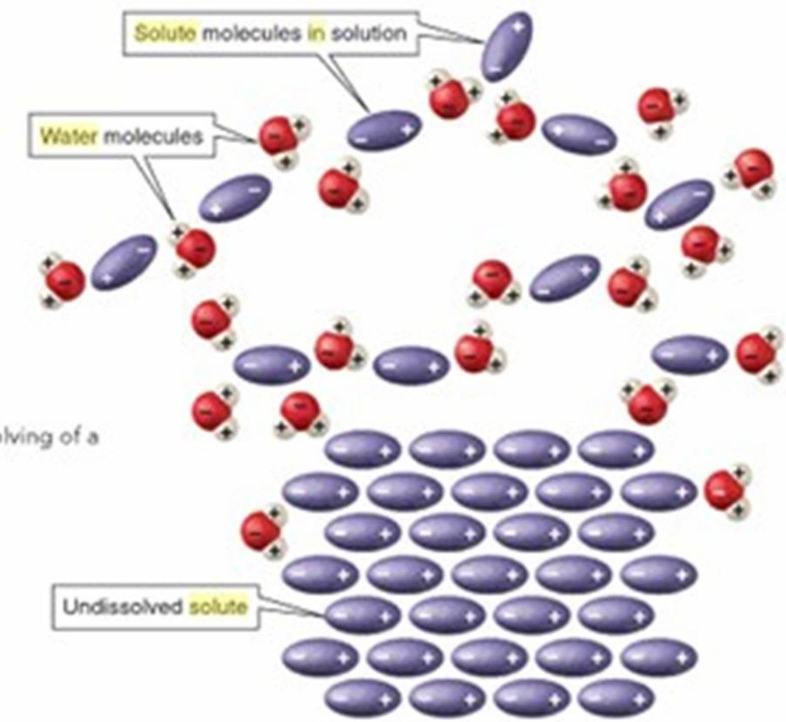
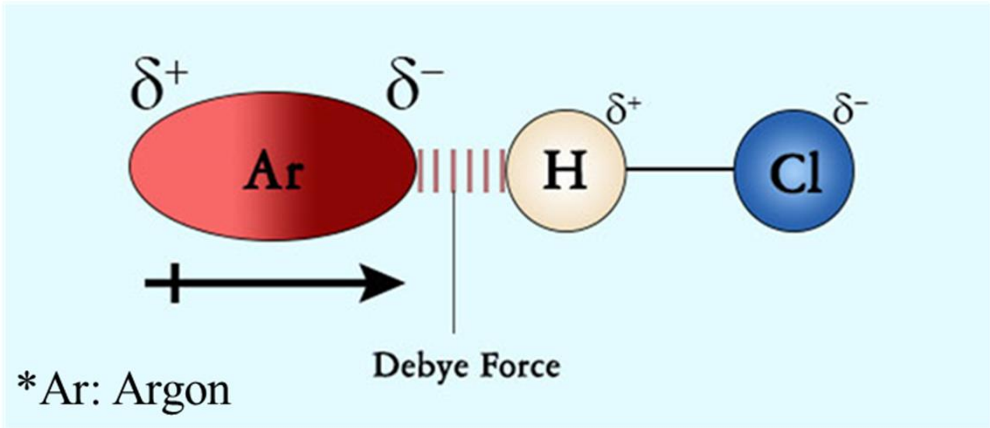
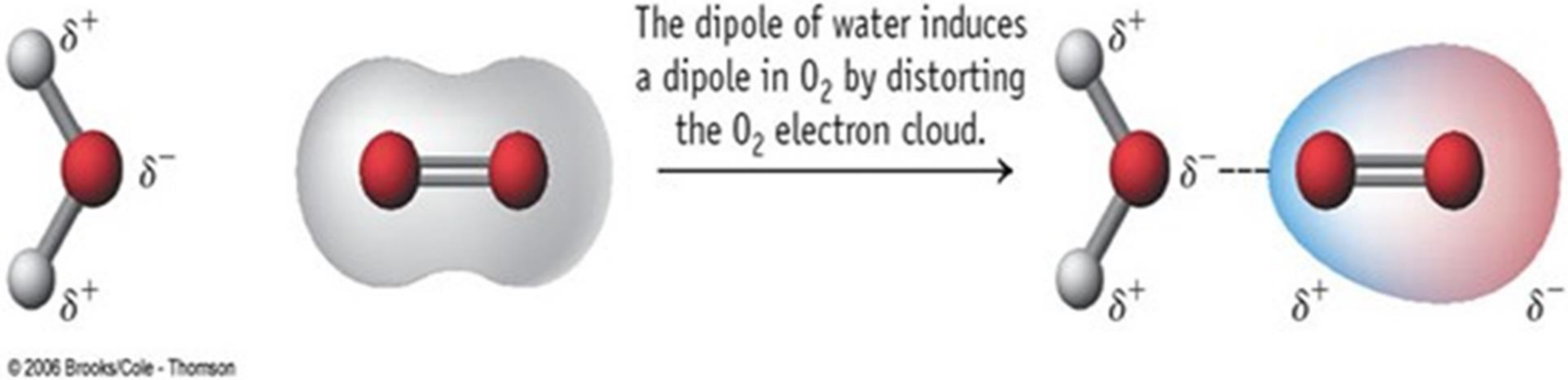


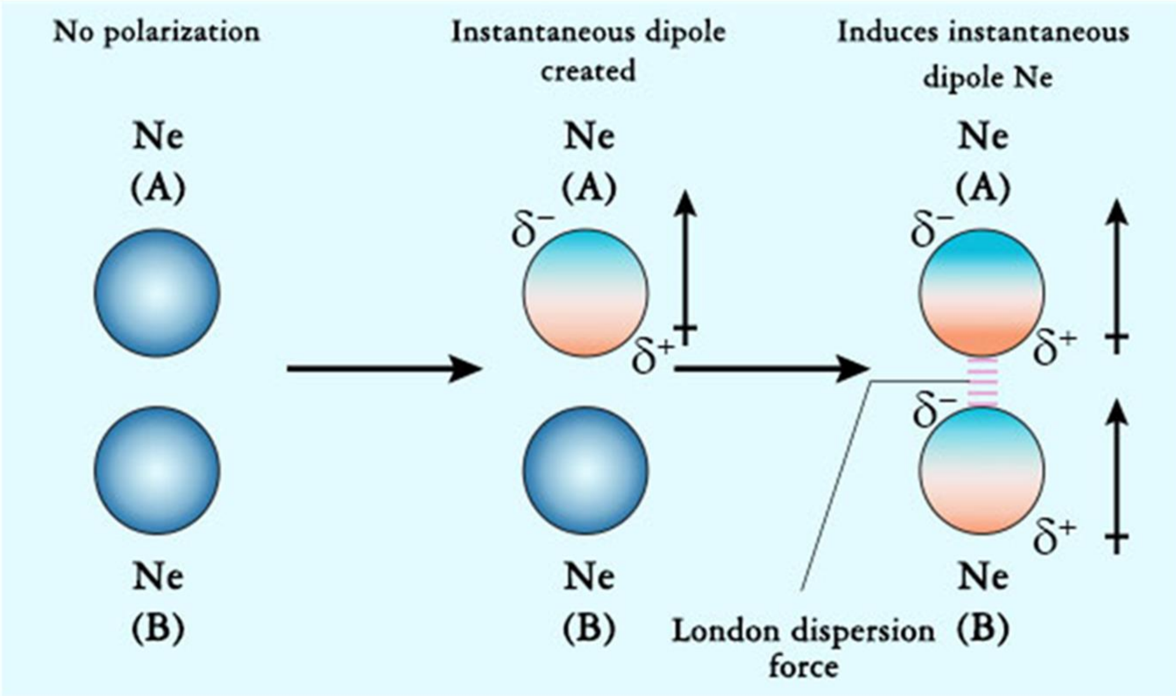
Figure 7.5 The dissolving of a polar solute in water.

VDW Forces: Debye Force
(Force btw a permanent dipole and a corresponding induced dipole)



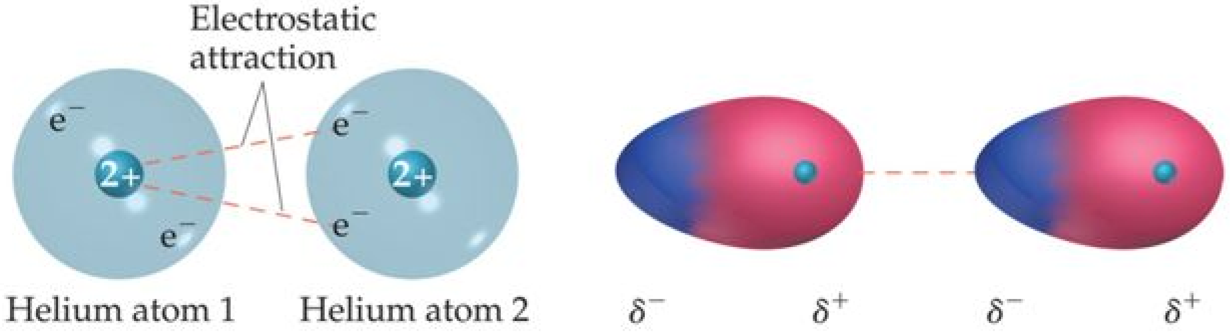


VDW Forces: London Dispersion Force



- Arises due to the instantaneous dipole that may be created in the atoms of molecules due to the movement of electrons.
  - As the electrons in an atom are in continuous motion, there might be an instance when most of the electrons have shifted to one side of the electron cloud causing a momentary dipole to be created.
  - When two such instantaneous dipoles come close together, there is attraction between the molecules.
- This is the weakest amongst all the forces, but is present in almost all molecules and atoms.

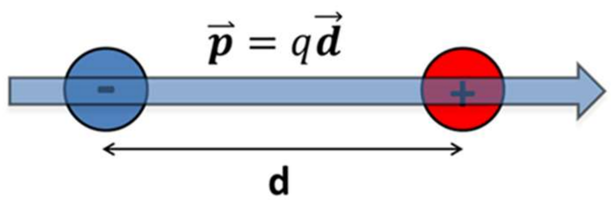
London Dispersion Forces

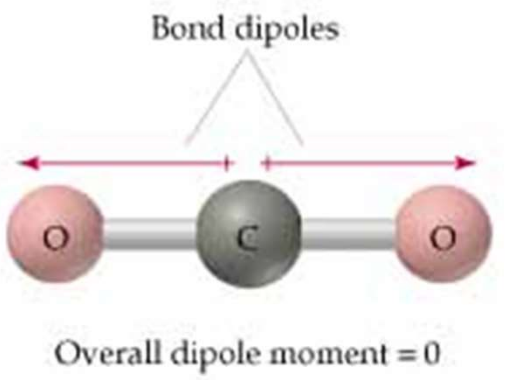


- These forces are present in *all* molecules, whether they are polar or nonpolar.
  – Only force present in nonpolar molecules
- The tendency of an electron cloud to distort in this way is called polarizability.
  – Polarizability increases with the number of electrons in the molecule, and is enhanced by the presence of pi bonds (multiple bonds)

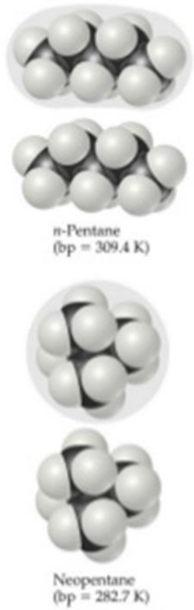
Dispersion Forces

- Are the forces that lead to **distortions in the electron clouds of an atom, by neighboring atoms or electrons**.
- The **more electronegative** atom of a molecule **will pull the electron density** of the **bond closer to itself**, gain itself a **partial negative charge** leaving the other atom **with a partial positive charge.**
  - Gives a **dipole moment** to a molecule.





Factors Affecting London Forces



- The shape of the molecule affects the strength of dispersion forces: long, skinny molecules (like n-pentane tend to have stronger dispersion forces than short, fat ones (like neopentane).
- This is due to the increased surface area in n-pentane.

Halogen	Molecular Weight (amu)	Boiling Point (K)	Noble Gas	Molecular Weight (amu)	Boiling Point (K)
F_2	38.0	85.1	He	4.0	4.6
Cl_2	71.0	238.6	Ne	20.2	27.3
Br_2	159.8	332.0	Ar	39.9	87.5
I_2	253.8	457.6	Kr	83.8	120.9
			Xe	131.3	166.1

- The strength of dispersion forces tends to increase with increased molecular weight.
- Larger atoms have larger electron clouds which are easier to polarize.

Relative strength of intermolecular f attraction

Intermolecular force	Occurs between …	
Dipole-dipole attraction	Partially oppositely charged ions	
Hydrogen bonding	H atom and O, N/ or	Str

How these forces of attraction affect properties of compounds?

Type of compound	Intermolecular forces present	Relative order of boiling and melting points
Ionic compounds	Ion to ion attraction between ions, London dispersion forces	1, highest)
Covalent compounds containing hydrogen bonds	Hydrogen bonds, London dispersion forces	2
Polar covalent compounds	Dipole-dipole attraction between dipoles created by partially charged ions, London dispersion forces	3
Nonpolar covalent compounds	London dispersion forces	4, lowest

- **The stronger the intermolecular forces of attraction, the more energy is required to break those forces.**
- This translates into ionic and polar covalent compounds having higher boiling and melting points, higher enthalpy of fusion, and higher enthalpy of vaporization than covalent compounds.

<table>
<tr><th colspan="2">Class</th><th>Unit 1</th><th>Unit 2</th><th>Energy (Kcal/mole)</th><th>bonding</th></tr>
<tr><td rowspan="3">Van der Waals forces</td><td>Keesom forces</td><td>Dipole</td><td>Dipole</td><td>1~7</td><td rowspan="6">Physical bonding (intermolecular interaction)</td></tr>
<tr><td>Debye forces</td><td>Dipole</td><td>Induced dipole</td><td>1~3</td></tr>
<tr><td>London forces</td><td>Induced dipole</td><td>Induced dipole</td><td>0.5~1</td></tr>
<tr><td colspan="2">Ion-dipoles forces</td><td>Ion</td><td>Dipole</td><td>1~7</td></tr>
<tr><td colspan="2">Ion-induced dipole forces</td><td>Ion</td><td>Induced dipole</td><td>-</td></tr>
<tr><td colspan="2">Hydrogen bond</td><td>H atom</td><td>O, N, F</td><td>2~8</td></tr>
<tr><td colspan="2">Ionic bond</td><td>Ion</td><td>Ion</td><td>100~200</td><td rowspan="2">Chemical bonding (atomic bonding)</td></tr>
<tr><td colspan="2">Covalent bond</td><td>Polar atom</td><td>Polar atom</td><td>50~150</td></tr>
</table>

References

1. GLASER R. Biophysics: An Introduction (2012). 2nd Ed. Springer.
2. COTTERIL R. Biophysics: An Introduction (2002). John Wiley & Sons.
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