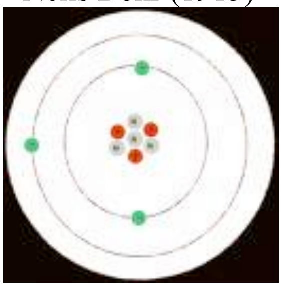
Atomic theory:

- Neils Bohr (1913) – won his Nobel prize for his atomic theory – NOT fully correct



- the neutrons (no charge) and protons (positively charged) occupy a dense central region called the nucleus
- the electrons (negatively charged) orbit the nucleus much like planets orbiting the Sun

- de Broglie (1924) – his 12 page PhD thesis won him the Nobel prize
  - he proposed that ordinary "particles" such as electrons and protons could behave as both particles and waves (wave-particle duality)

Particles $\leftrightarrow$ Waves

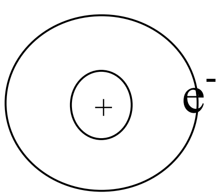
- the orbitals of an atom are described by wave functions (mathematical equations) – they have no direct physical meaning but when squared, provide electron density
- ψ = orbital
- ψ^2 = (orbital) ^{2} = electron density distribution

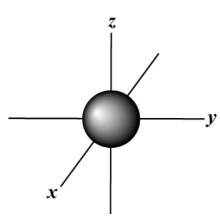
Note. Often the electron density distribution is called an "orbital" by chemists

For hydrogen (H) atom: >95% of electron density is found within 1Å = 10^{-8} cm

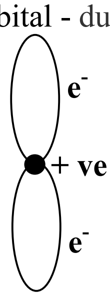
Orbitals:

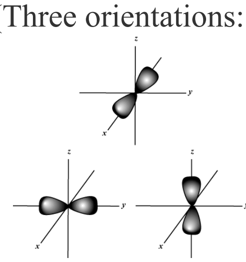
1. S-orbital - spherical shaped (electron density)





2. p-orbital - dumbbell-shaped (Three orientations: placed on the x, y and z-axis)





Basic principles:

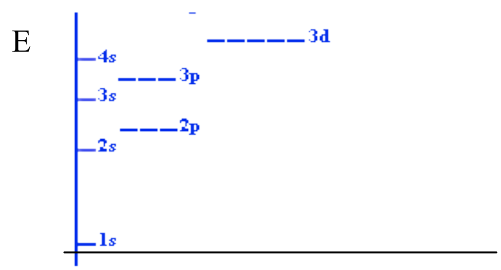
- like charges repel each other; while unlike charges attract each other
- atoms want to be in inert gas electron configuration (isoelectronic with inert gas; such as He, Ne, Ar,.. Helium is the inert gas that Hydrogen can be isoelectronic with)

Atoms	Protons (+)	Neutrons	1s electrons	2s electrons	2p electrons
H	1	0	1		
He	2	2	2		
Li	3	3	2	1	

Abbreviation of electron - e^-

Mass Number = (Number of Protons) + (Number of Neutrons)

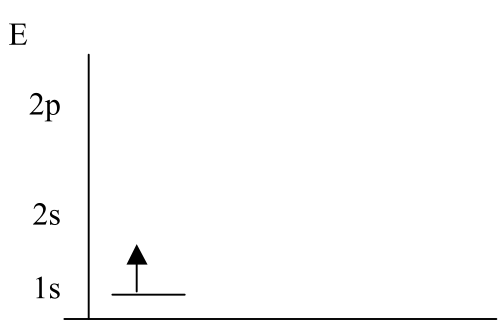
Energy (E) level diagram for an atom:



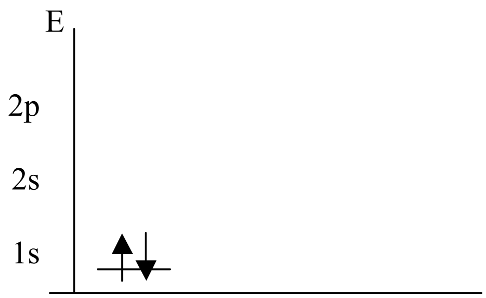
Rules for filling electron – AUFBAU rule (Build up Principle):

- add electron to lowest energy orbital available
- maximum two electron per orbital (each having opposite spin quantum number)
- Pauli Exclusion principle
- fill 1 electron into each orbital of same energy (degenerate orbital), then add second electron – Hund's rule

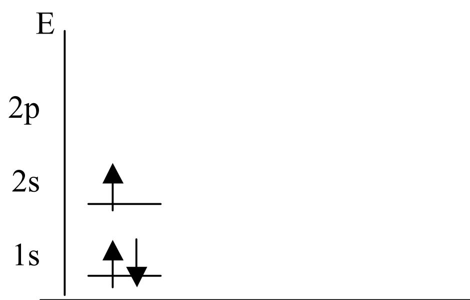
Hydrogen (H)



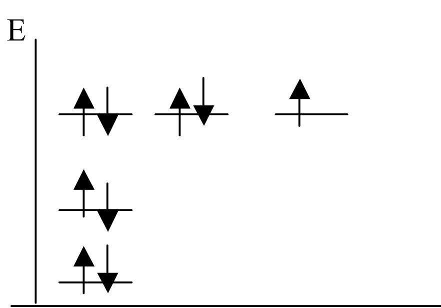
Helium (He)



Lithium (Li)



Fluorine (F)



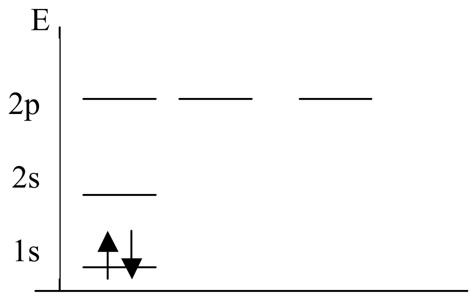
- all elements want inert gas configuration (e.g. Ne) and from above diagrams both Li and F are unhappy with unfilled orbitals (not in inert gas configuration)

Bonding - Ionic

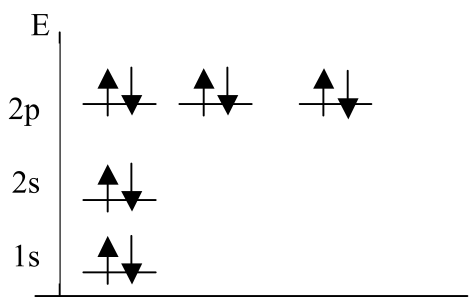
- isoelectronic = same electron configuration
- Li could lose 1e$^-$ from 2s orbital to be isoelectronic to He (as Li^+) and F could gain 1e$^-$ to be isoelectronic to Ne (as F^-)

$$Li^o + F^o \rightarrow Li^+ + F^-$$

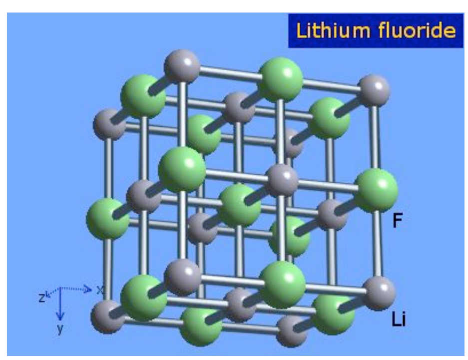
Li^+ (cation)



F^- (anion)



- in space these ions would be attracted to each other
- in solution they might be separated due to solvation (e.g. water would surround)
- in solid, they would form a crystalline solid structure



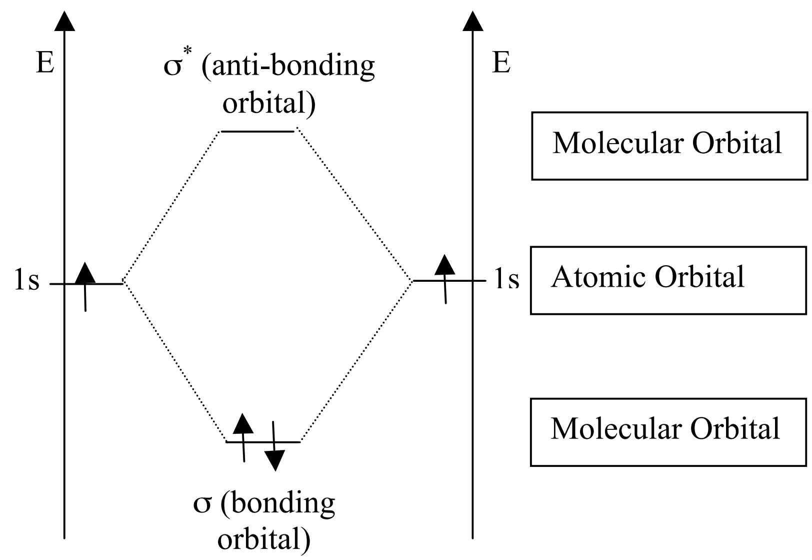
Lithium fluoride is an example of Ionic bonding in which positive and negative species are bounded to each other.

Covalent Bonding

- Sharing of electrons between the atoms.

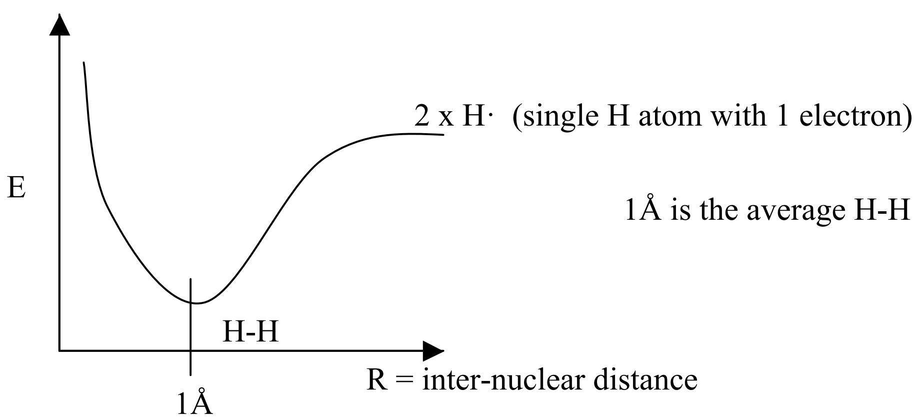
Energetics of Forming Bonds

e.g) H_2



e.g As these two hydrogen atoms come together

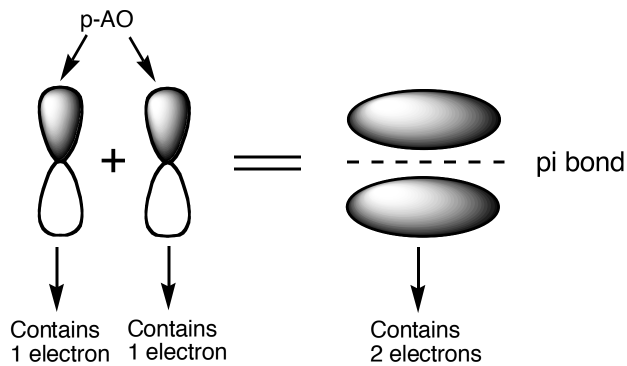
$H^{\cdot} \longrightarrow H{:}H \longleftarrow {}^{\cdot}H$



1Å is the average H-H bond distance

<u>**Linear Combination of Atomic Orbitals (LCAO)**</u>

- Gives molecular orbitals (MO)
- Overlap of s atomic orbitals (AO) → gives sigma(σ) MO (cylindrical symmetry)
- Overlap of p AO → gives pi(π) MO



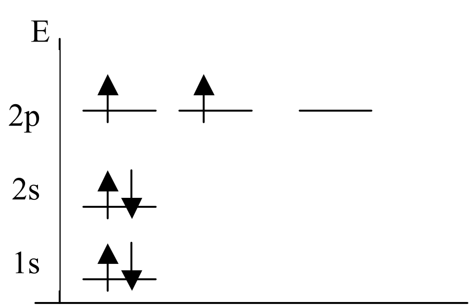
- Difference between AO and MO → AO present on an atom while MO present between two atoms when bond is formed.

In terms of strength → σ bond is stronger than a π bond. But a double bond is stronger than a single bond because double bonds contain two bonds (σ-bond + π-bond).

Electronic configuration of carbon (C):

- atomic number = 6
- atomic weight = 12
- other isotopes of carbon
    - ^{13}C ($6p^+$, 7n) is a stable isotope, 1% natural abundance
    - ^{14}C ($6p^+$, 8n) is radioactive, $t_{1/2}$ = 5700 yrs, ^{14}C dating of organic material

Carbon (C)



- need to gain or lose $4e^-$ to get inert gas configuration – but this gives unfavourable charge buildup:

- C^{4+} isoelectronic with He

- C^{4-} isoelectronic with Ne

- so, carbon makes 4 bonds to share $4e^-$ (covalent bonding)

Hybridization:

- mixing of atomic orbitals (with wrong geometry for bonding) to form the hybrid orbitals with the correct geometry for bonding

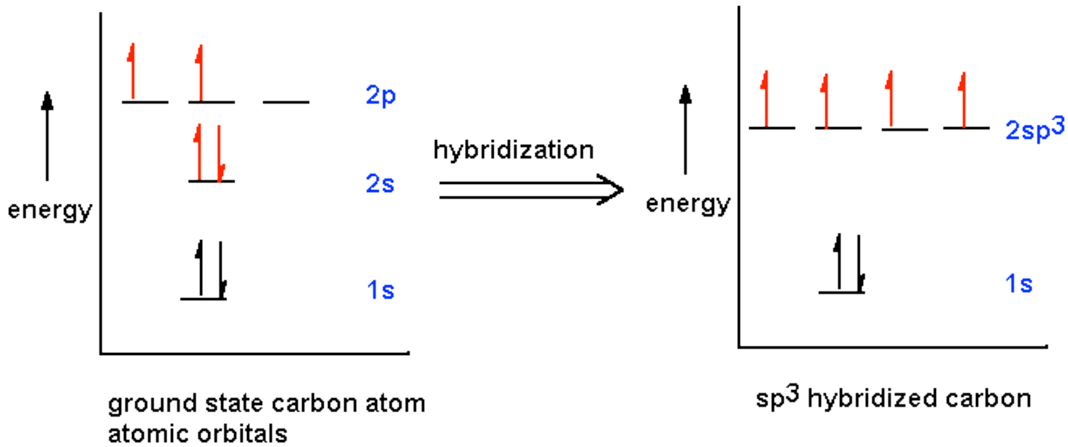
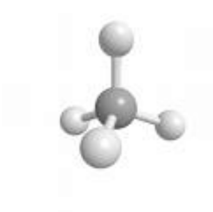


Figure: Hybridization of 2nd shell s (one) orbitals and p (three) orbitals of carbon

- So 1 (2s) orbital + 3 (2p) orbitals = 4 (sp^3) hybridized orbital
- the 2s orbital and 2p orbitals of carbon are mixed (hybridized) to form the four degenerate sp^3 orbitals
- note: sp^3 comes from the fact that one s-orbital and three p-orbitals are mixed
- once the hybrid orbitals are formed, four hydrogen atoms can share the four electrons of the outer (bonding) shell of carbon to form four covalent bonds
- now, carbon is isoelectronic to neon and hydrogen is isoelectronic to helium

e.g.

Methane, CH_4:



- tetrahedral geometry
- electron density is equidistance from nucleus
- four covalent bond between the carbon atom and the hydrogen atoms
- the angle between two H-atoms = 109°