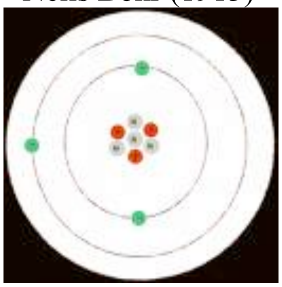
Atomic Theory:

- Neils Bohr (1913) – Won the Nobel prize for his atomic theory – <u>NOT fully correct</u>



- 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 ↔ Waves

Often the electron density distribution is called an "orbital" by chemists
- The orbitals of an atom are described by wave functions (mathematical equations)
- These have no direct physical meaning, but when squared describe electron density

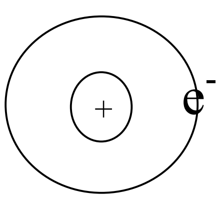
ψ = orbital

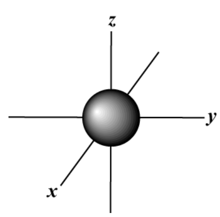
ψ^2 = (orbital) ^{2} = electron density distribution

For the hydrogen (H) atom: >95% of electron density is found in a sphere with diameter of 1Å (10^{-8} cm)

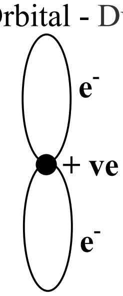
Orbitals:

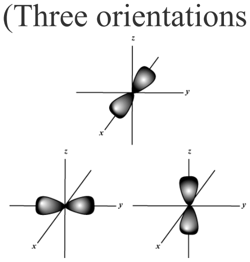
1. *s*-Orbital - Spherical shaped (electron density)





2. *p*-Orbital - Dumbbell-shaped (Three orientations: placed on the x, y and z-axis)





Basic Principles:

- Like charges repel each other; unlike charges attract each other
- Atoms want to have an inert gas electron configuration (isoelectronic with inert gas, such as He, Ne, Ar. Helium is the inert gas that hydrogen can be isoelectronic with)

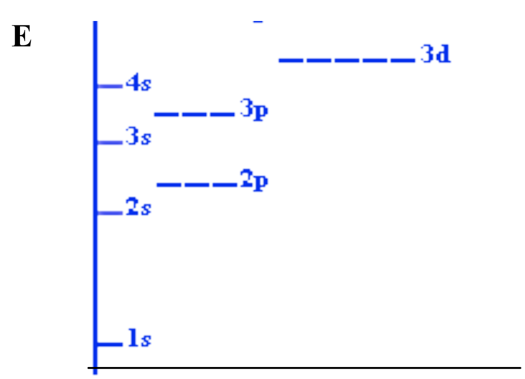
Atoms	Protons (+) = Atomic #	Neutrons	1s electrons	2s electrons	2p electrons
H	1	0	1		
He	2	2	2		
Li	3	3	2	1	

Rules for Filling Electron Orbitals – AUFBAU Rule (Building-Up Principle):

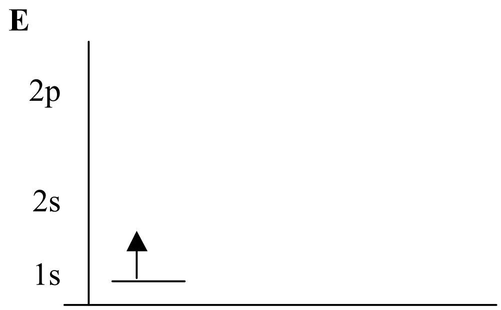
1) Add electron to the lowest energy orbital available
2) Maximum of two electron per orbital (each having opposite spin quantum number)
    - Pauli Exclusion Principle
3) Place one electron into each orbital of the same energy (degenerate orbitals), before adding a second electron
    - Hund's Rule of Maximum Multiplicity

Abbreviation of electron: $\mathbf{e^-}$
Mass Number = (Number of Protons) + (Number of Neutrons)
Atomic Number – Number of Protons

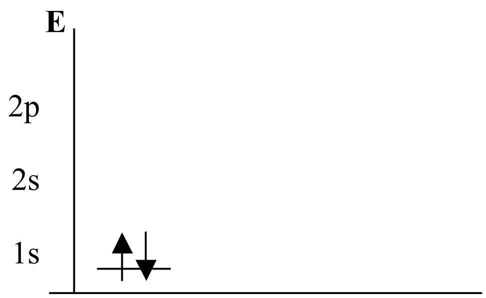
Energy (E) Level Diagram for an Atom:



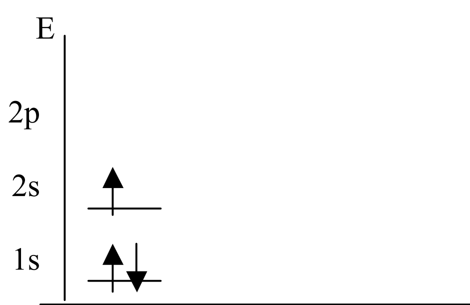
Hydrogen (H)



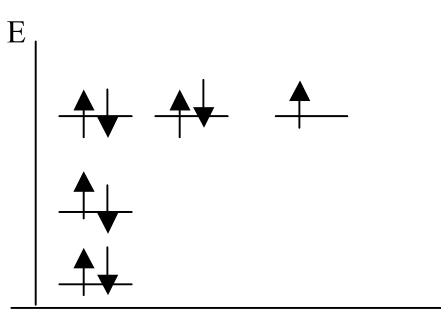
Helium (He)



Lithium (Li)



Fluorine (F)



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

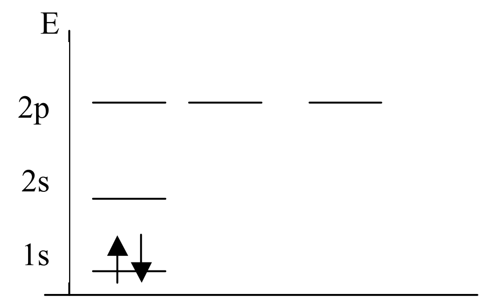
Ionic Bonding

Lithium fluoride is an example of ionic bonding in which positive and negative species are bonded to each other. Li could lose 1e$^-$ from 2s orbital to become isoelectronic to He (as Li$^+$) and F could gain 1e$^-$ to become isoelectronic to Ne (as F$^-$).

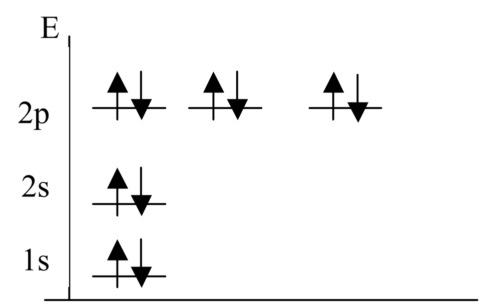
$$Li^o + F^o \rightarrow Li^+ + F^-$$

Isoelectronic = Same electron configuration

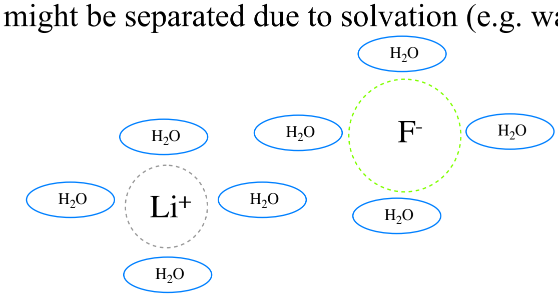
Li$^+$ (cation) Isoelectronic with He



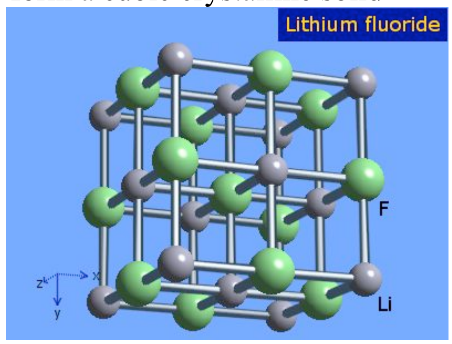
F$^-$ (anion) Isoelectronic with Ne



In space, Li$^+$ and F$^-$ would be attracted to each other
In solution, Li$^+$ and F$^-$ might be separated due to solvation (e.g. water would surround)



In a solid, Li^+ and F^- would form a cubic crystalline solid

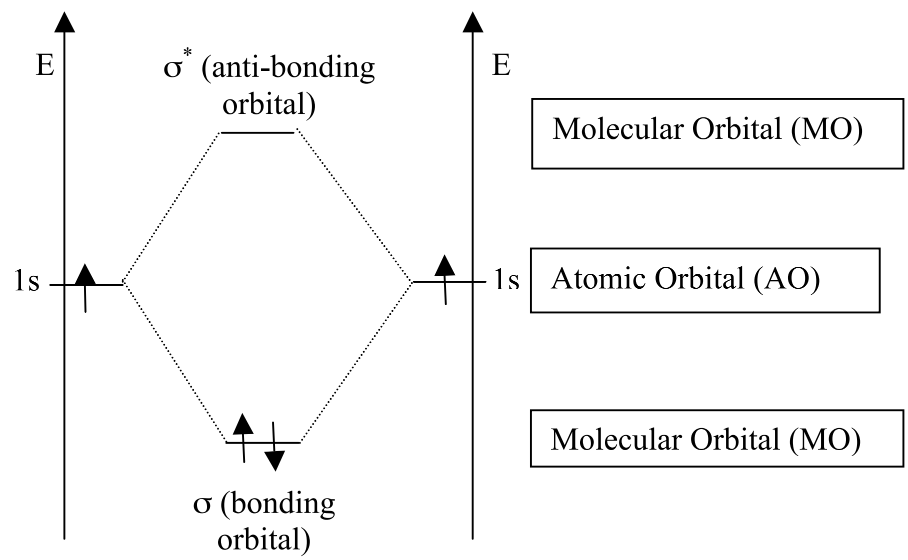


Covalent Bonding

- Sharing of electrons between the atoms
- More common in organic chemistry

Energetics of Forming Bonds

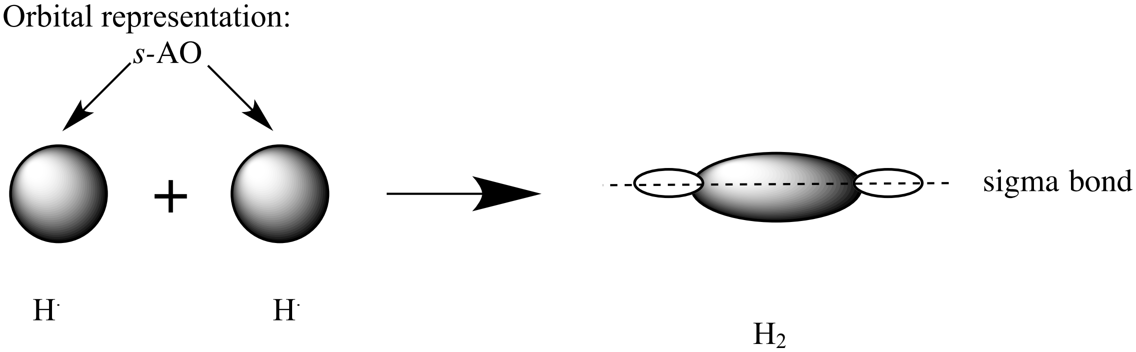
e.g. H_2



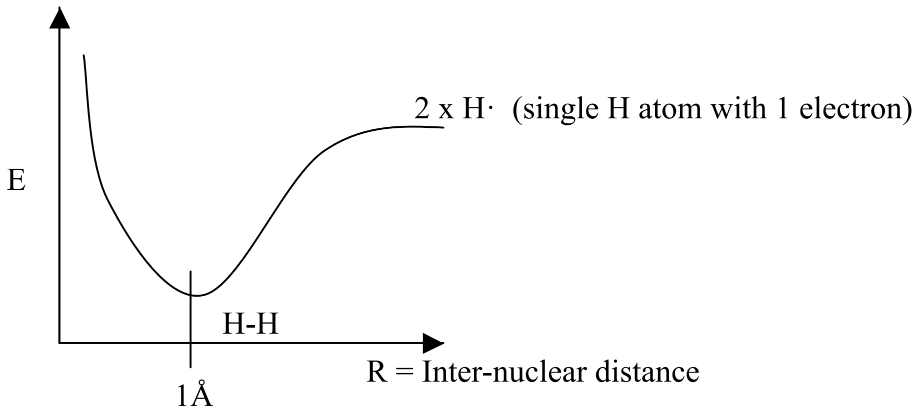
As these two hydrogen atoms come together, molecular hydrogen (H_2) is formed

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

Orbital representation:



Energy diagram of two hydrogen atoms interacting to form a bond:

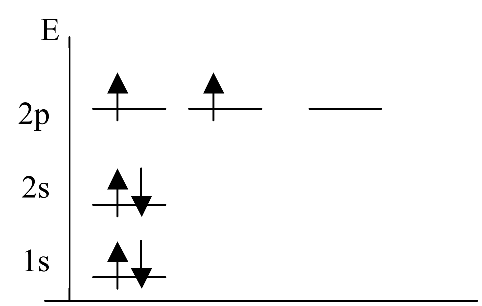


1Å is the average H-H bond distance

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)



- Carbon needs to gain or lose $4e^-$ to get an inert gas configuration, but this would result in unfavourable charge buildup:

- C^{4+} is isoelectronic with He

- C^{4-} is isoelectronic with Ne

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

Hybridization:

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

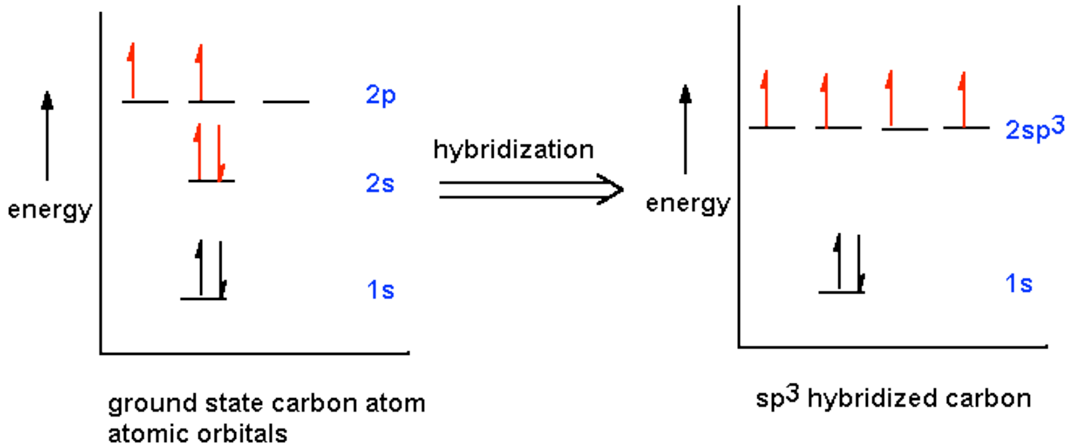
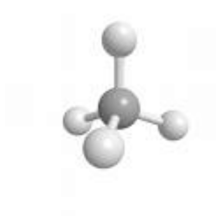


Figure: Hybridization of 2nd shell *s* (one) orbitals and *p* (three) orbitals of carbon

Note: sp^3 comes from the fact that one s-orbital and three p-orbitals are mixed

- 1 (2*s*) orbital + 3 (2*p*) orbitals = 4 (sp^3) hybridized orbitals
- The 2*s* orbital and 2*p* orbitals of carbon are mixed (hybridized) to form four degenerate (of the same energy) sp^3 orbitals
- 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
- After bonding, carbon is isoelectronic to neon and hydrogen is isoelectronic to helium

Methane, CH_4:



- Tetrahedral geometry
- Electron density is equidistance from nucleus
- Four covalent bonds between the carbon atom and the hydrogen atoms
- The angle between two H-atoms = 109°