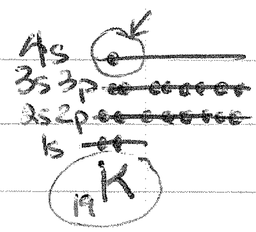
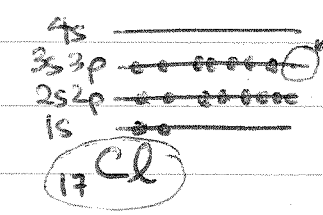
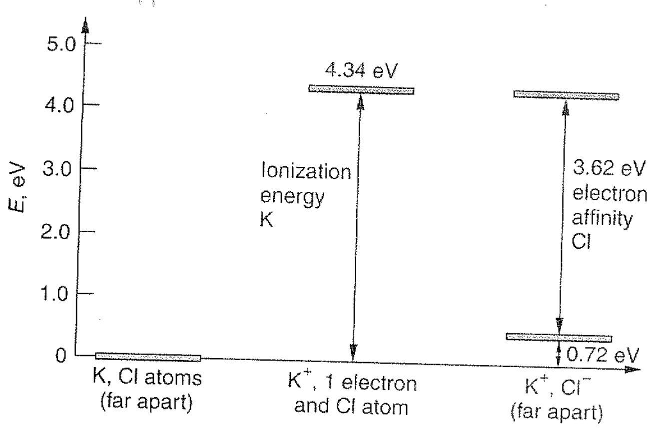
Chemical Bonding

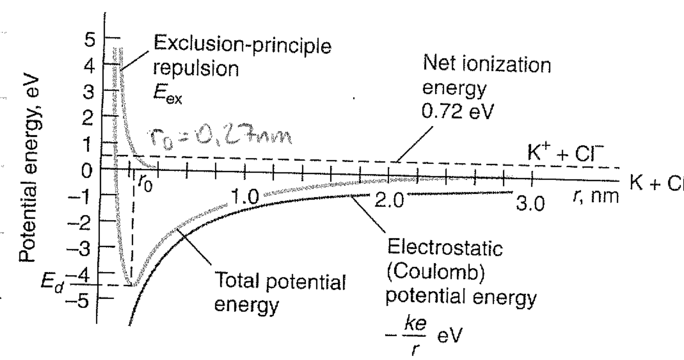
- * molecule is the smallest chemical unit.
- * bonding involves sharing e^- between atoms
  to overcome the Coulomb repulsion
- * tightness of bonds is limited by Pauli repulsion
- * ignore inner electrons, protons & neutrons in nuclei, etc.
  only construct Molecular Orbitals (MO) for VALENCE electrons.
- * bond types: A) IONIC B) COVALENT C) DIPOLE-DIPOLE D) METALLIC
- * common feature: minimization of energy.

Ionic Bond





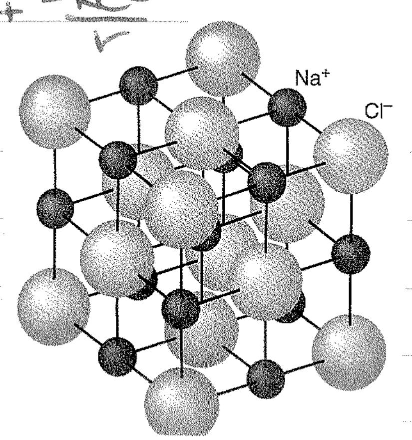




$$U(r) = E_{ion} + E_{ex} + E_c = E_{ion} + \frac{A}{r^n} + \frac{-ke^2}{r}$$

minimum at: $r = r_0$ bond length

$U(r_0) = E_d$ dissociation energy.



$$U_{att} = -\alpha \frac{ke^2}{r} \qquad \alpha = 6 - \frac{12}{\sqrt{2}} + \frac{8}{\sqrt{3}} - \frac{6}{2} + \frac{20}{\sqrt{5}} - \cdots \qquad \textbf{10-2}$$

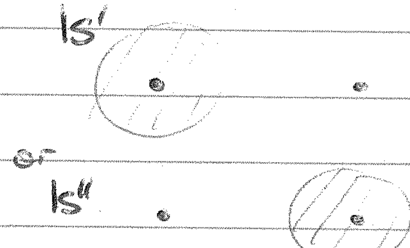
Covalent Bond

- see Wikipedia: Molecular orbital.

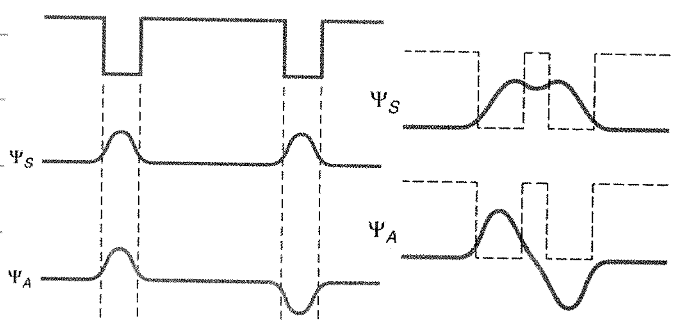
MO * molecular orbital: Friedrich Hund (1927) & Robert S. Mulliken (1928)

LCAO * linear combinations of atomic orbitals: Sir John Lennard Jones (1929)

* adapt atomic orbitals to the symmetry of the molecule.
  - much like n-particle wave functions of indistinguishable particles
    i.e. Pauli Exclusion principle.
  - now: 2+ particles (e^-) and 2+ nuclei
* energy splitting as 2 H-atoms come closer together:
* example: H_2 molecule.

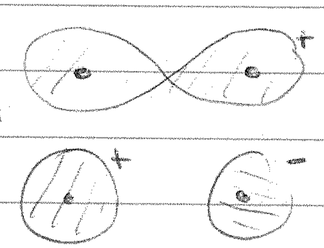


single-particle states

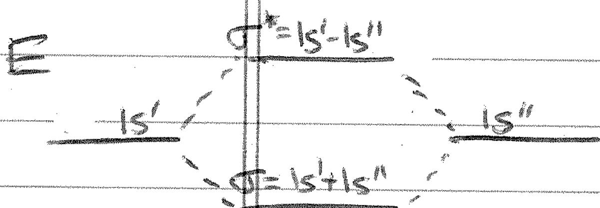


$\sigma = 1s' + 1s''$ bonding "covalent bond"

$\sigma^* = 1s' - 1s''$ anti bonding



symmetrized states.



spin: ↑↓ in σ orbital.
↑↑ in σ* orbital (already antisymmetric).

H : H

$\text{bond order} = \dfrac{\#\text{bonding electrons} - \#\text{antibonding electrons}}{2}$

* example: He_2: 4 electrons fill 2 sym + 2 antisym states → no bonding

Dipole-Dipole Bond

- 2 dipoles: $E_d \sim 1/r^3$
- polar-nonpolar: e.g. hydrogen bond - snowflakes
- nonpolar: $E_d \sim 1/r^6$ induced polarization Van der Waals Force

Metallic Bond

- analog of covalent bond in an atomic lattice
- many-electron states split to form dense band of states