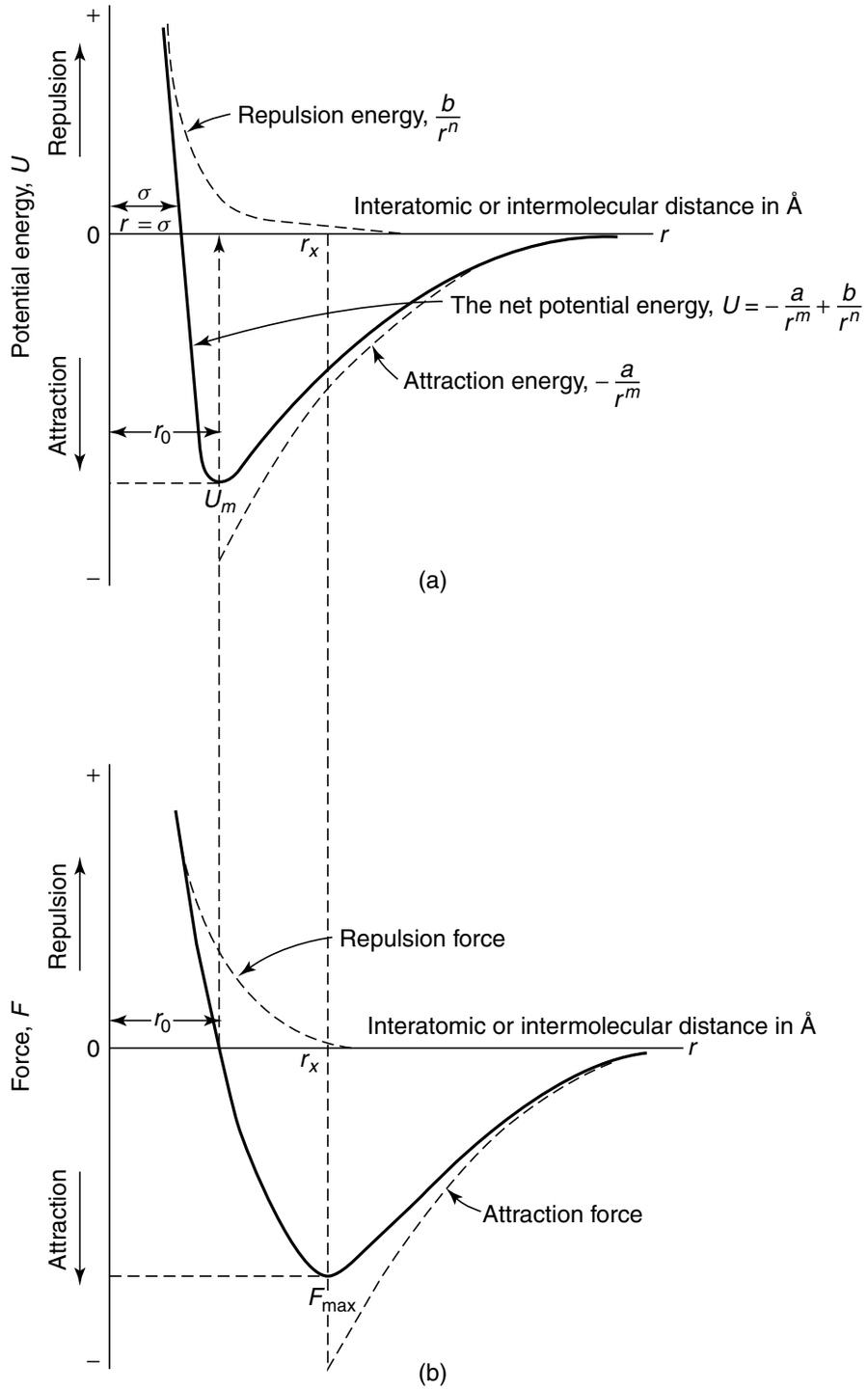
Bonding



Mie potential

$$U = U_a + U_r = \frac{-a}{r^m} + \frac{b}{r^n}$$

$$U = U_a + U_r = \frac{-a}{r^6} + \frac{b}{r^{12}}$$

$$r_0 = \left(\frac{nb}{ma}\right)^{\frac{1}{n-m}}$$

Ionic Bond, Coulomb interaction

$$U=\left[\frac{Z_1 Z_2 e^2}{4\pi\varepsilon\varepsilon_0 r}\right] \qquad U=\left[\frac{a}{r^m}\right]$$

Can we build the repulsive term

$$r_0=\left(\frac{nb}{ma}\right)^{\frac{1}{n-m}}$$

Here we know m=1

$$U_0 = \frac{z_1 z_2 e^2}{4\pi\varepsilon\varepsilon_0}\left(\frac{1}{1} - \frac{1}{n}\right)\frac{1}{r_0}$$

Our derived bond energy

$$\grave{u} = \frac{Q^2}{8\pi\varepsilon\varepsilon_0 a}$$

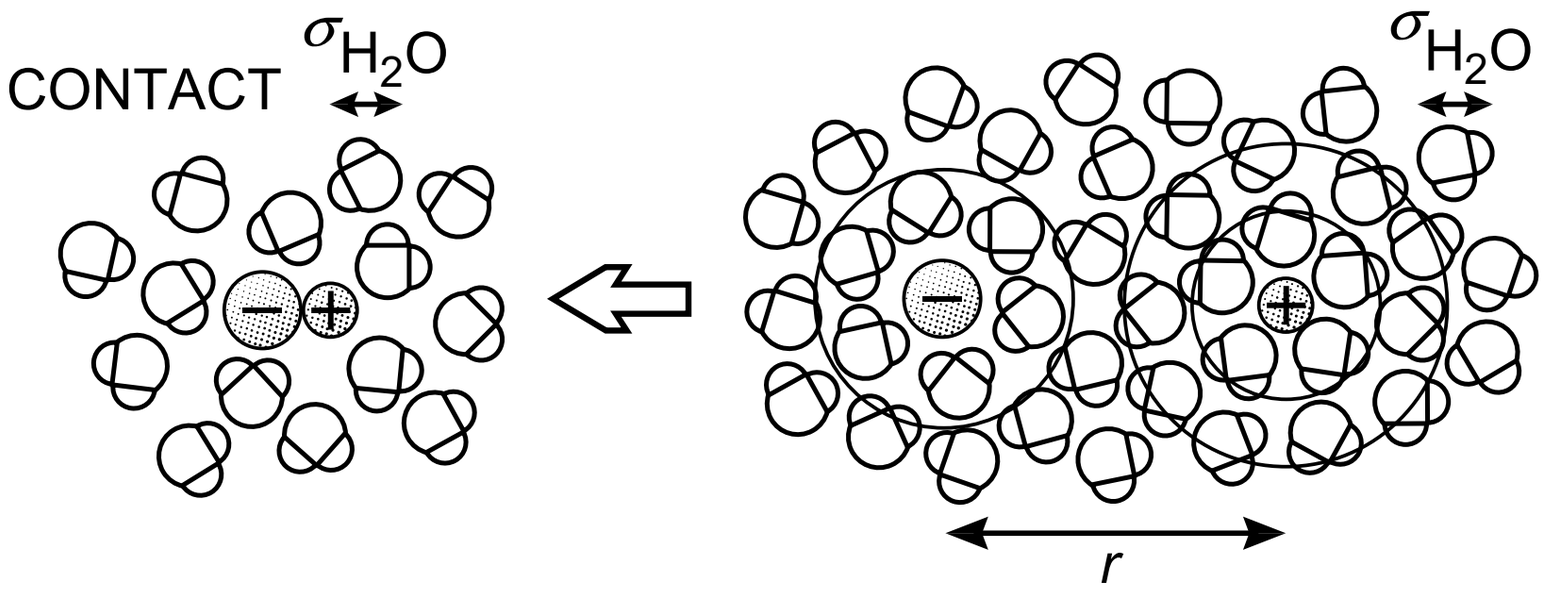
Born Self Energy

$$\Delta\grave{u} = \frac{Z^2 e^2}{8\pi\varepsilon_0 a}\left[\frac{1}{\varepsilon_1} - \frac{1}{\varepsilon_2}\right]$$

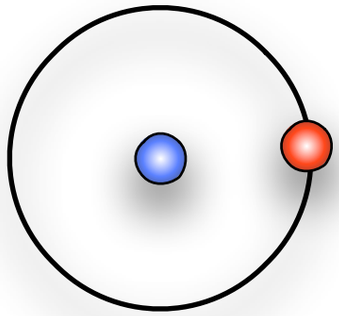
Self energy difference due to medium

$$\chi_s = e^{\frac{-\Delta\grave{u}}{KT}} = e^{-\left(\frac{z^2 e^2}{8\pi\varepsilon\varepsilon_0(a_+ + a_-)KT}\right)}$$

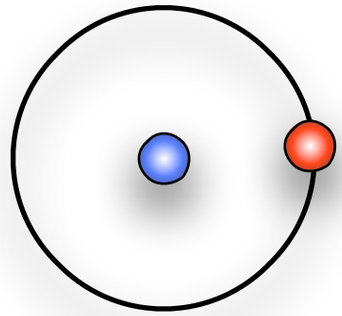
Solubility


CONTACT
σ_{H_2O}
σ_{H_2O}
r

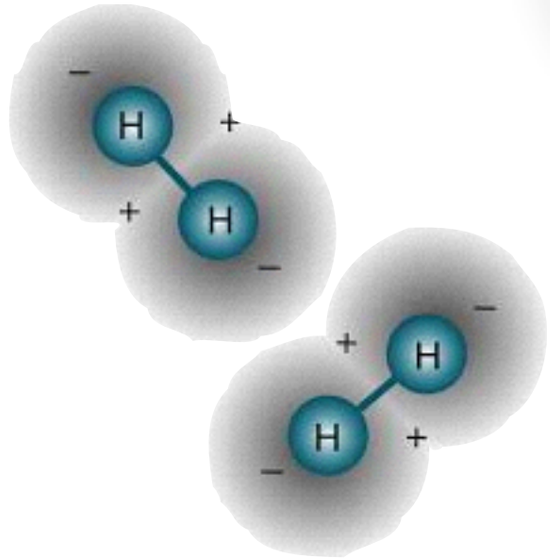
Covalent bonding



Hydrogen



Hydrogen



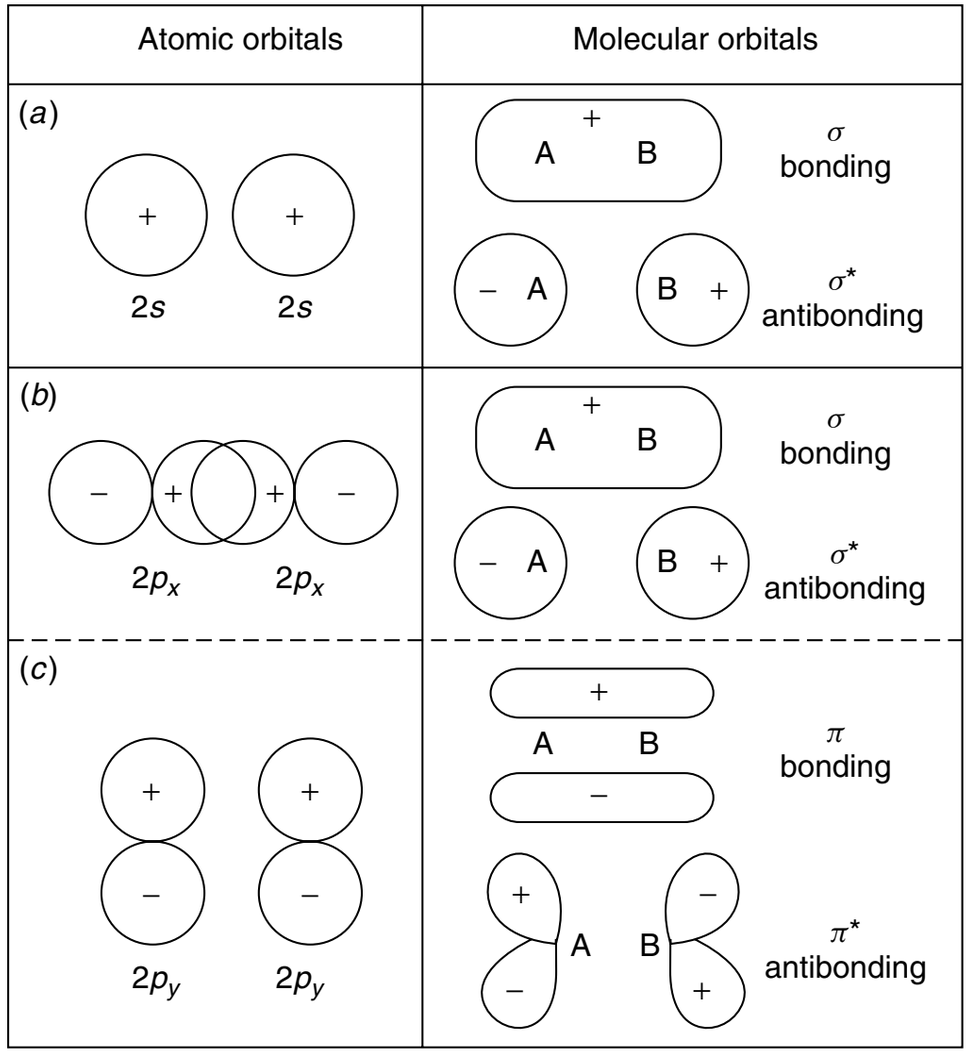


Figure 1.5 The shape of selected molecular orbitals formed from the overlap of two atomic orbitals. From K. M. Ralls, T. H. Courtney, and J. Wulff, *Introduction to Materials Science and Engineering*. Copyright © 1976 by John Wiley & Sons, Inc. This material is used by permission of John Wiley & Sons, Inc.

Example Oxygen

HF

Hydrogen

Flourine

Energy

σ^*

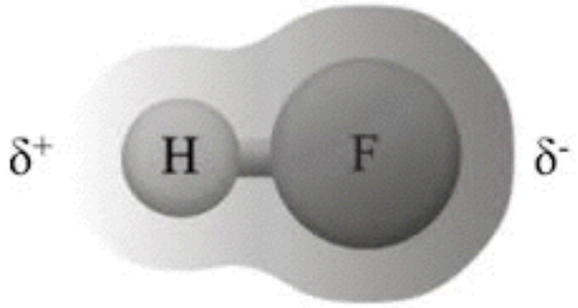
1s1 = -1310 kJ/mol

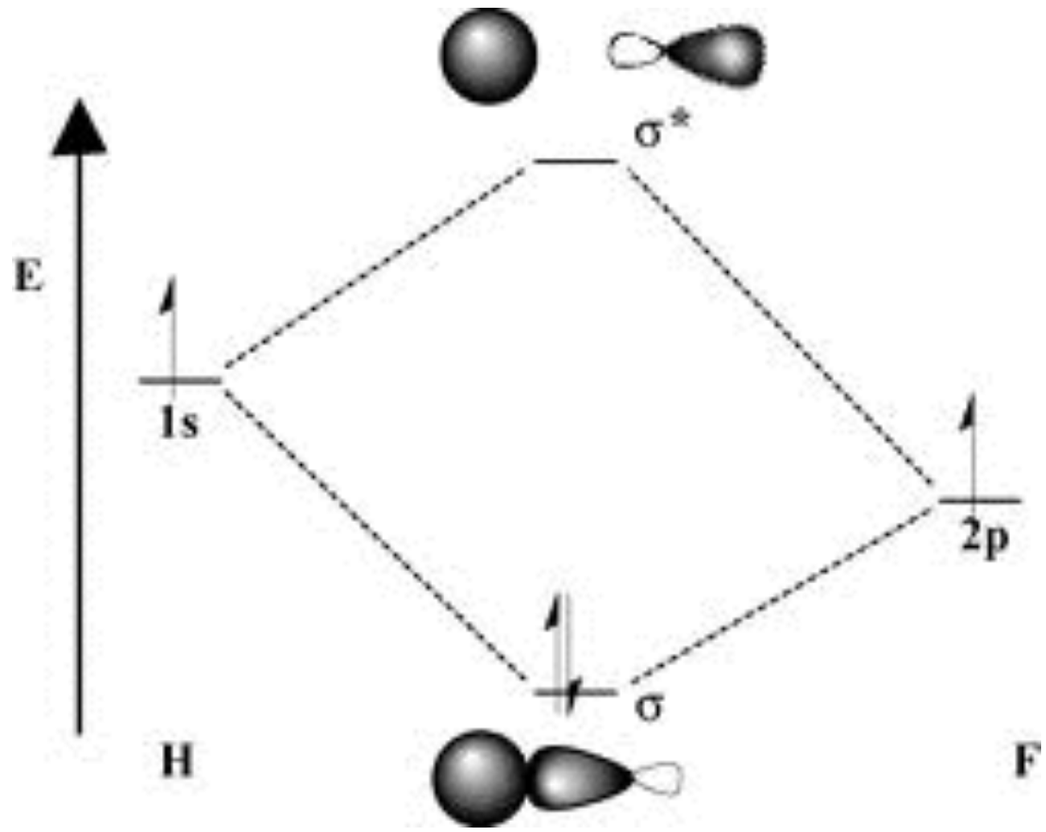
σ

2p5=-1682

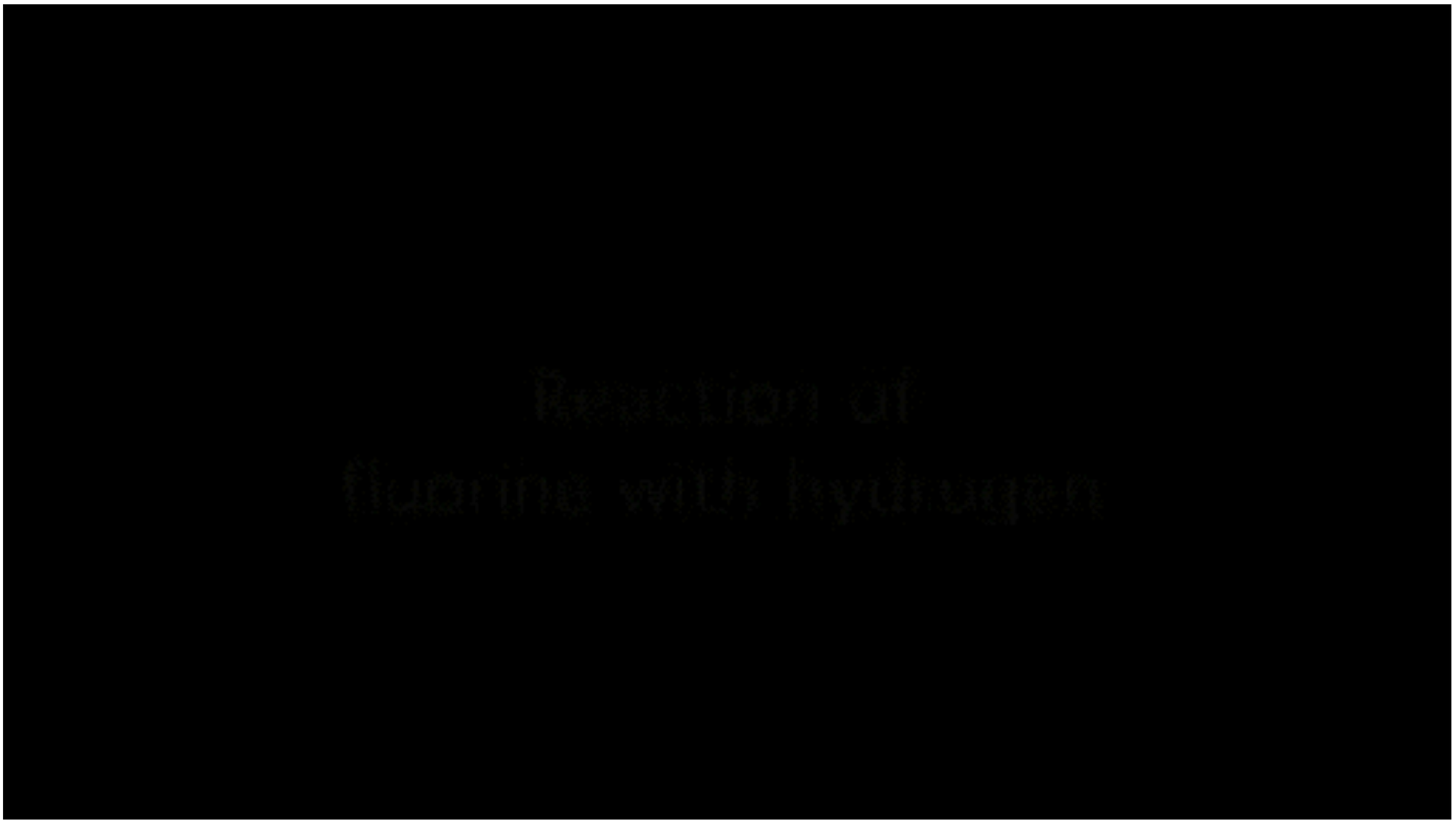
2s2

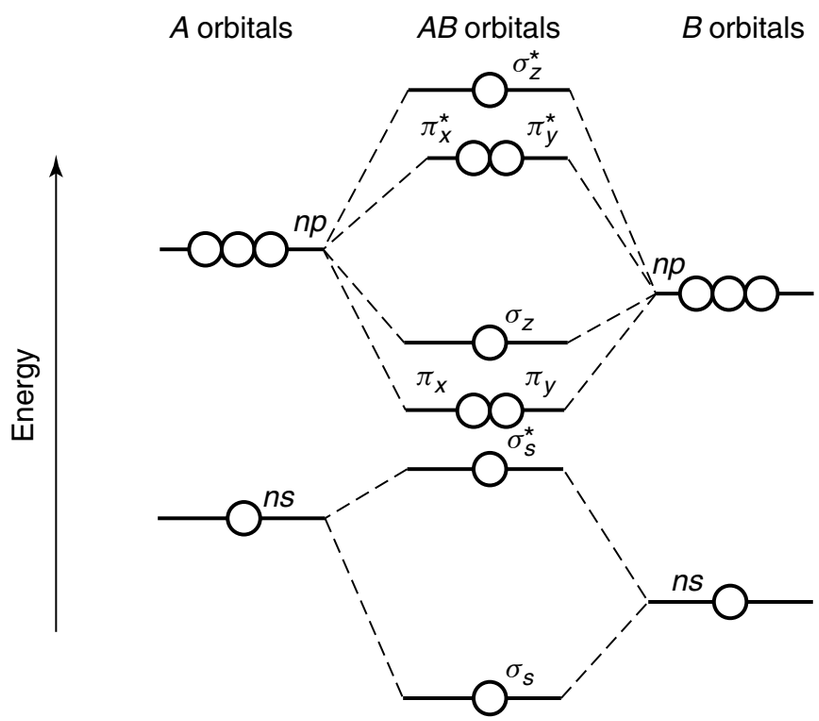
1s2





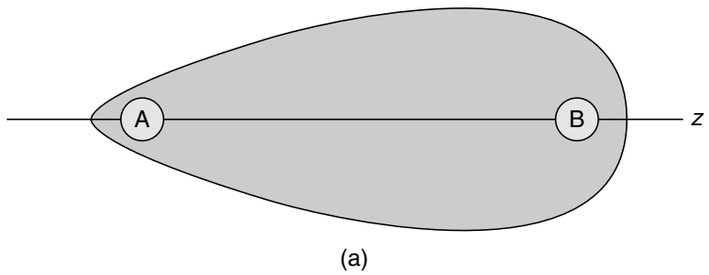
Formation of a polar molecule



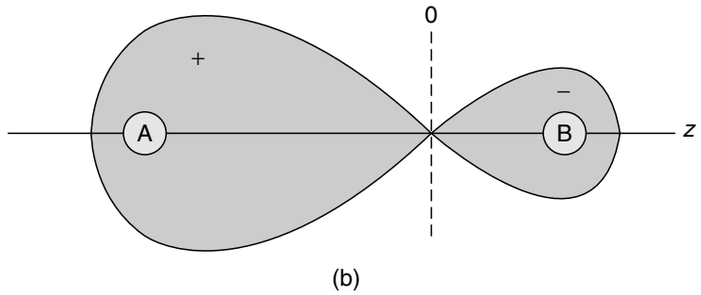


general AB molecule

Bonding Sigma



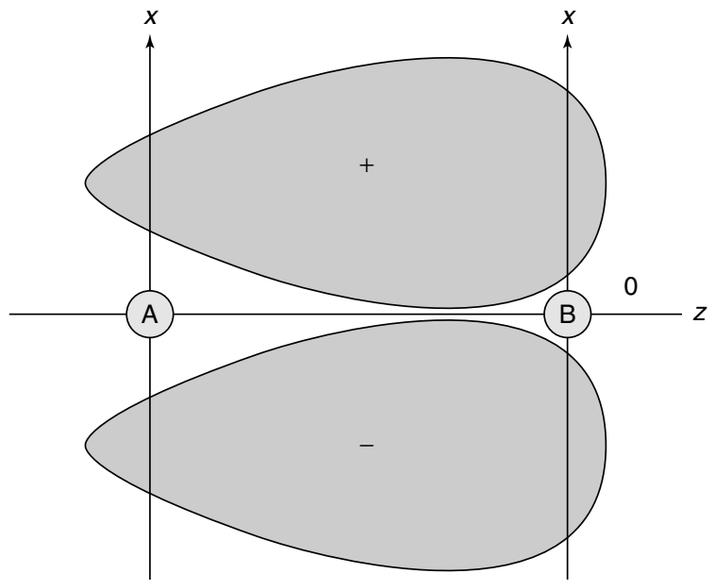
(a)



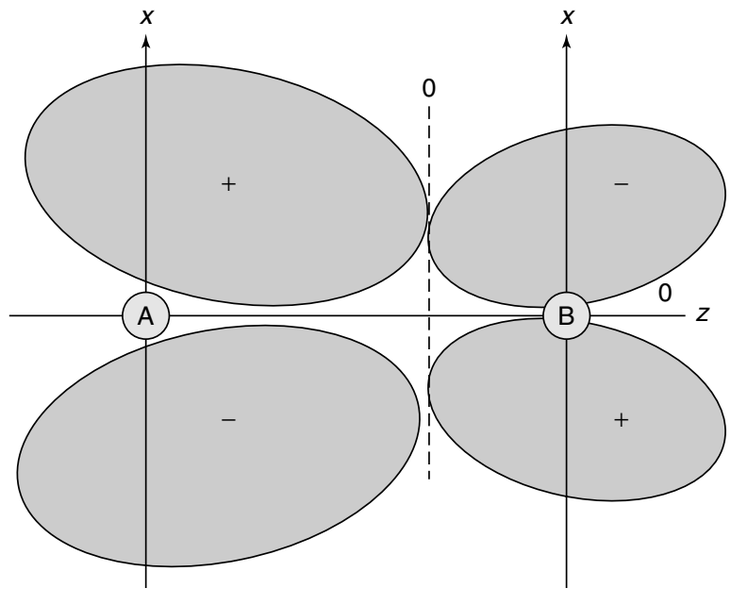
(b)

Anti Bonding Sigma

Anti Bonding Pi



(c)



(d)

Anti Bonding PI