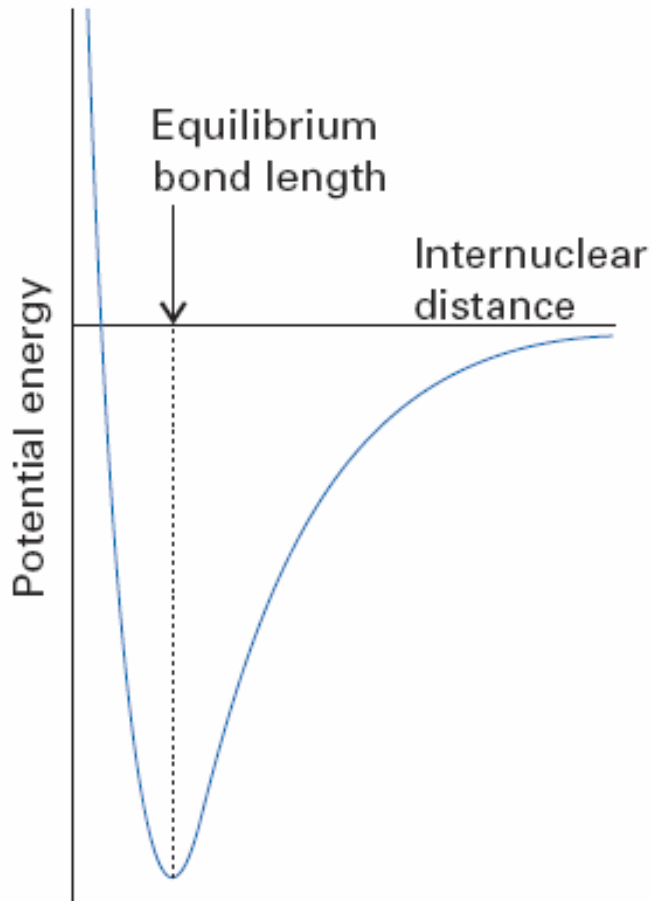# Chemical Bond

Born-Oppenheimer Approximation

Fig. 8.1 A typical molecular potential energy curve for a diatomic species.

- **The nuclei are much more massive than the electrons and hence move much slower**
- **Thus nuclei can be considered stationary while electrons move in their field**
- **We think of nuclei remaining fixed at arbitrary locations and then solve the Schrödinger equation for the wavefunctions of the electrons alone**
- **The molecular potential energy curve (adjacent figure) is so called because the kinetic energy of the stationary nuclei is zero.**
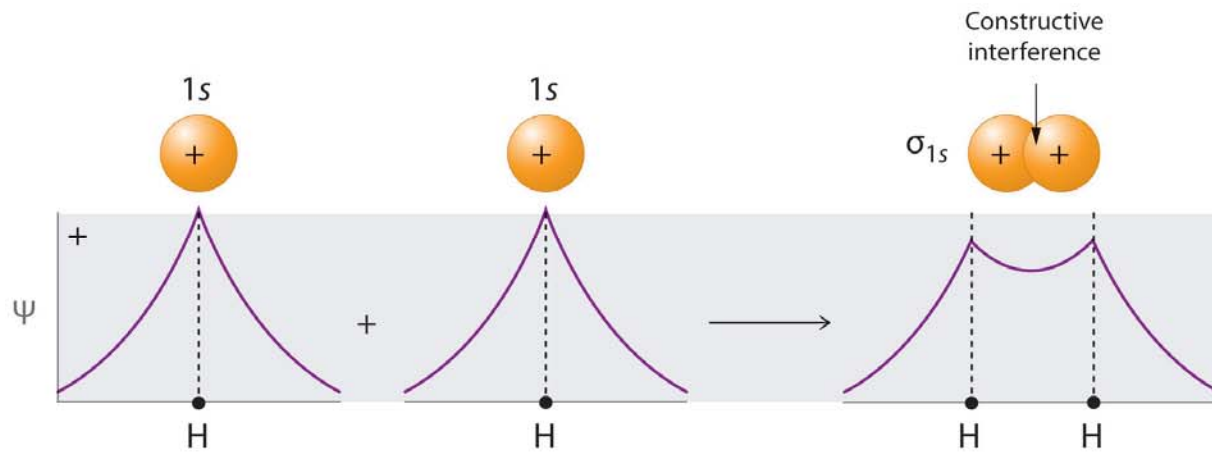
Hydrogen molecule ion wave functions

The spatial wavefunction on each of two H atoms forms linear combinations:

Ψ_{H1sA} or $1s_A$

Ψ_{H1sB} or $1s_B$

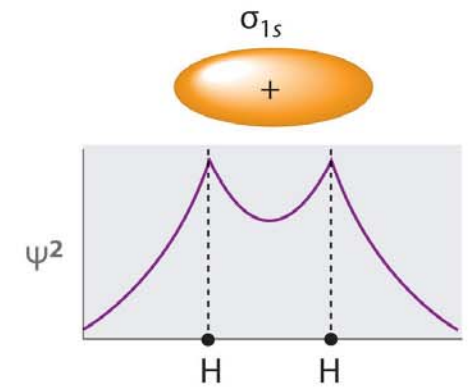e^-

r_A

r_B

R

A

B
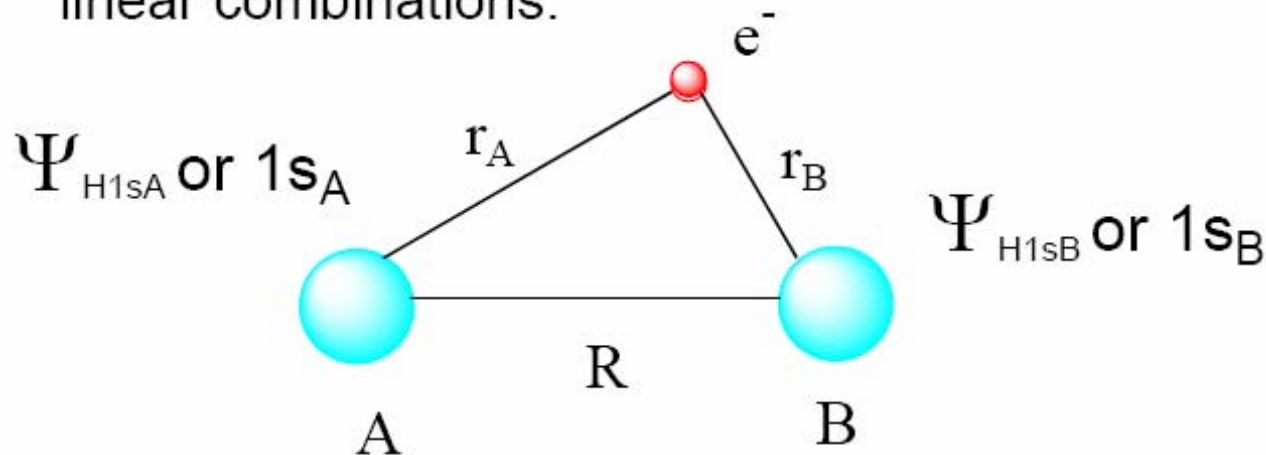
The atomic wave functions form linear combinations to make molecular orbital wave functions.
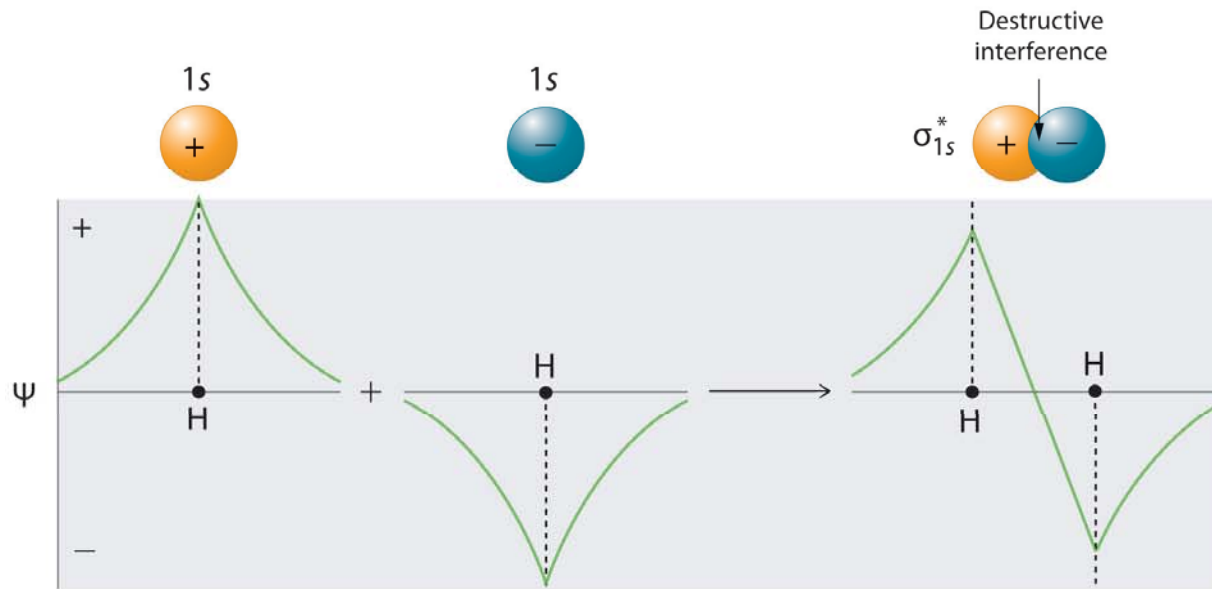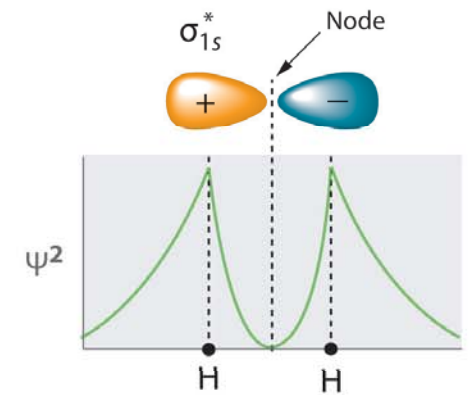
$$Y_\pm = 1s_A \pm 1s_B$$

(a) Wave functions combined for σ_{1s}

(b) Bonding probability density

(c) Wave functions combined for σ_{1s}^*

(d) Antibonding probability density
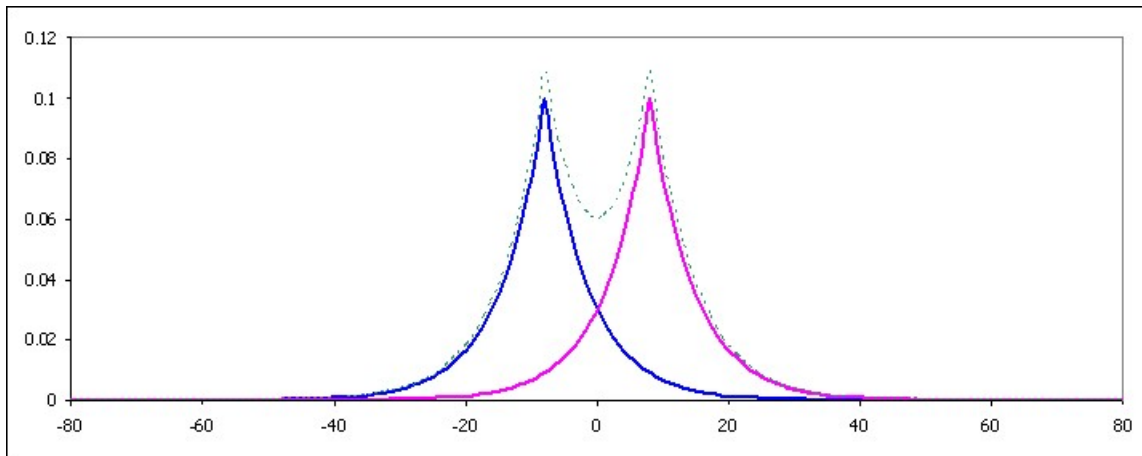
Diagram of H_2^+ energy levels

$$\frac{J - K}{1 - S}$$

anti-bonding

E_{1s} E_{1s}

bonding

$$\frac{J + K}{1 + S}$$
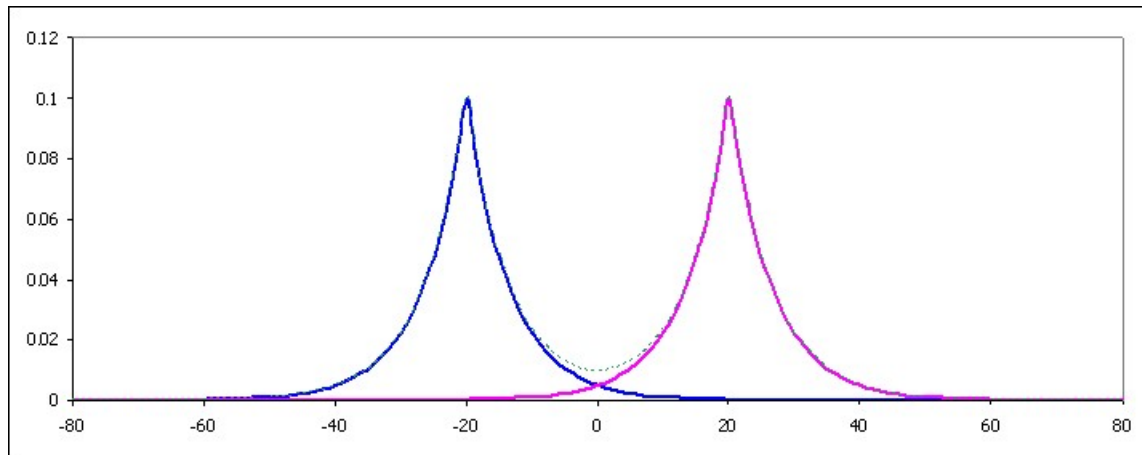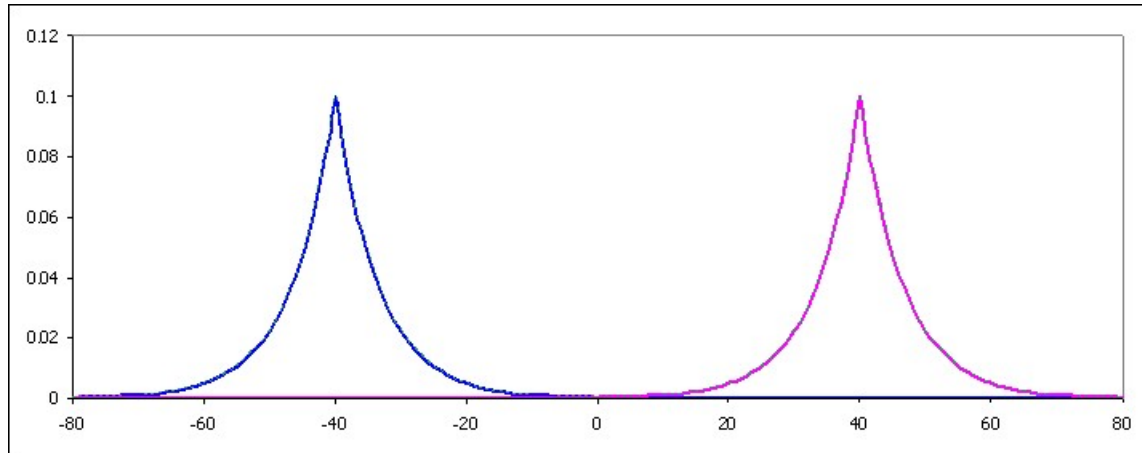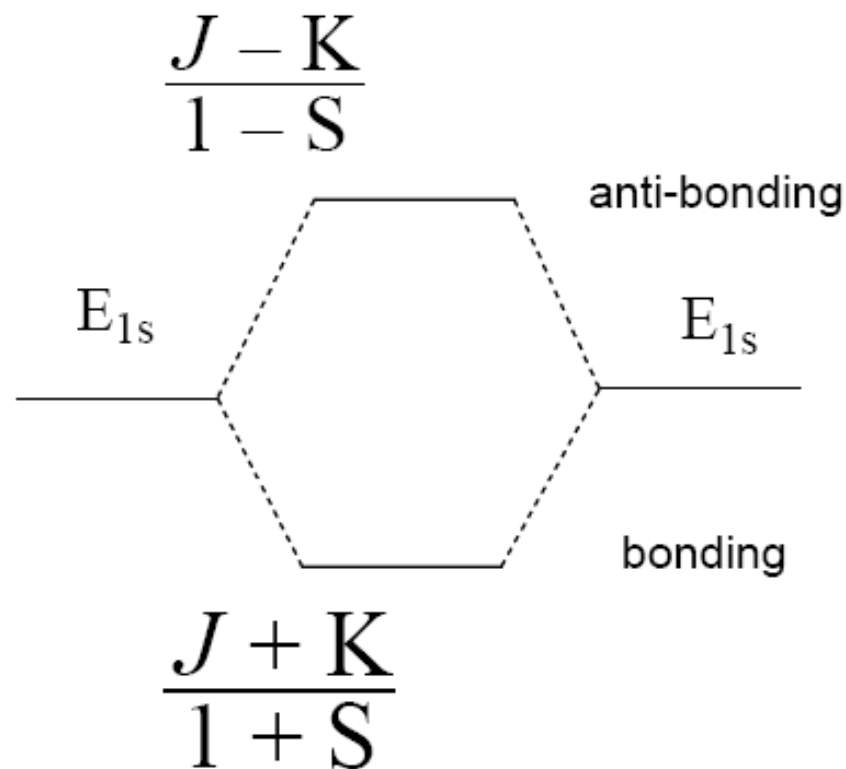
Note that the anti-bonding level is more destabilizing than the bonding level is stabilizing.