1.12

Electron Waves and Chemical Bonds

Models for Chemical Bonding

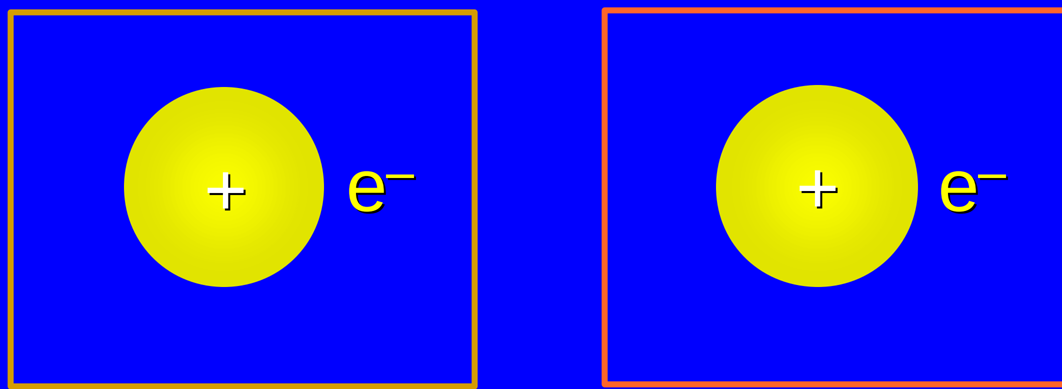
The Lewis model of chemical bonding predates the idea that electrons have wave properties.

There are two other widely used theories of bonding that are based on the wave nature of an electron.

Valence Bond Theory

Molecular Orbital Theory

Formation of H_2 from Two Hydrogen Atoms

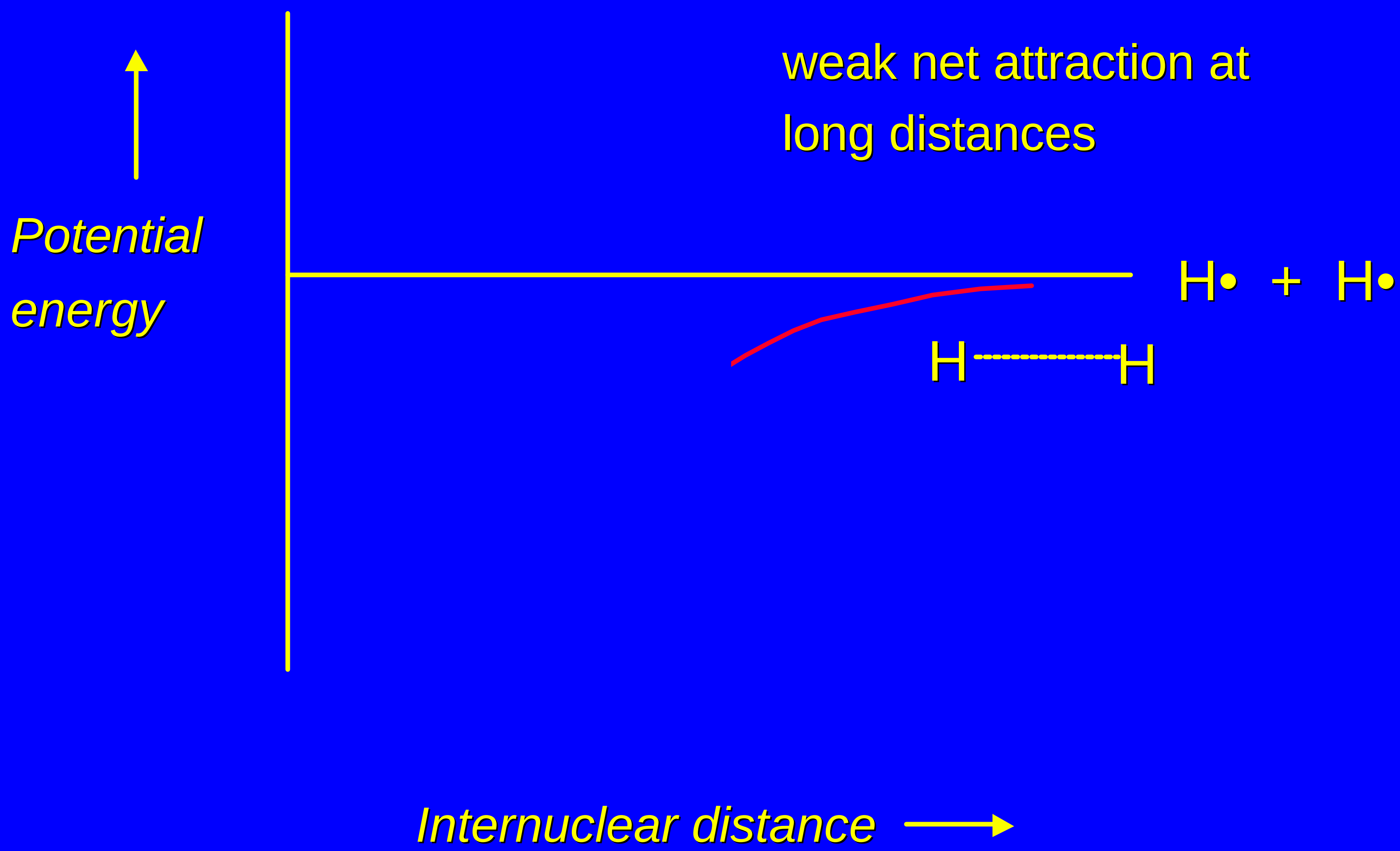


Examine how the electrostatic forces change as two hydrogen atoms are brought together.

These electrostatic forces are:

- attractions between the electrons and the nuclei
- repulsions between the two nuclei
- repulsions between the two electrons

Figure 1.14



weak net attraction at long distances
Potential energy
H• + H•
H-----------H
Internuclear distance

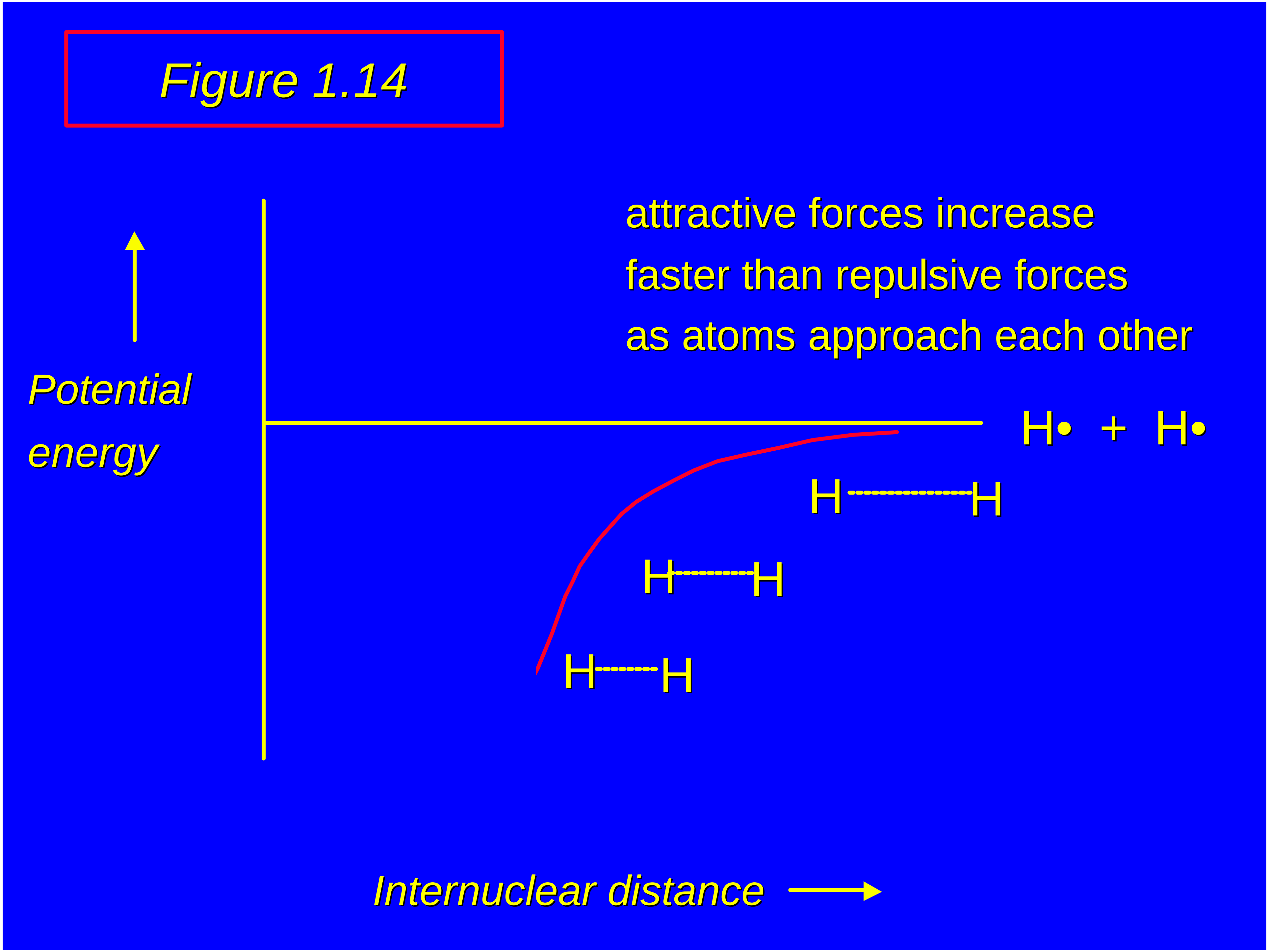


Figure 1.14
attractive forces increase
faster than repulsive forces
as atoms approach each other
Potential
energy
H• + H•
H-----------H
H--------H
H------H
Internuclear distance

Figure 1.14

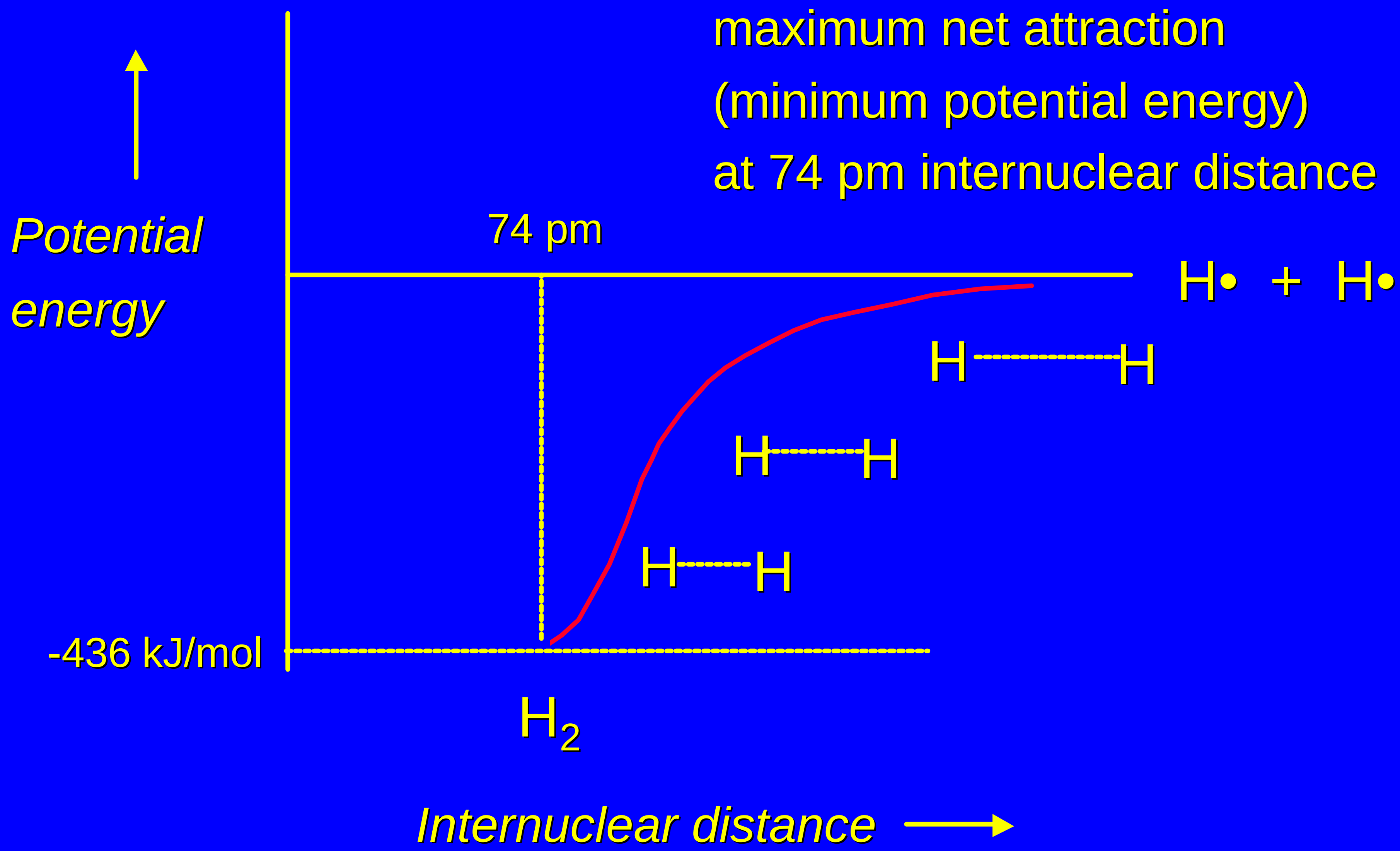
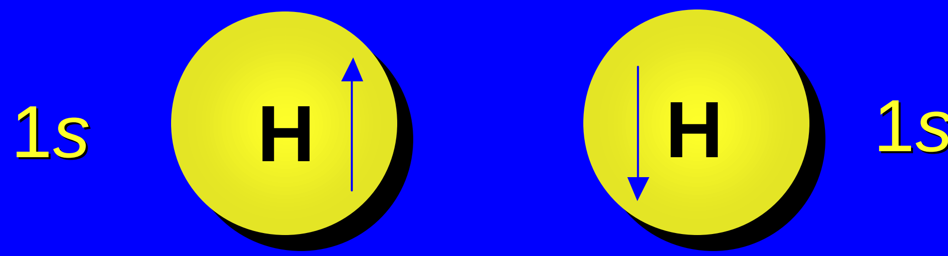
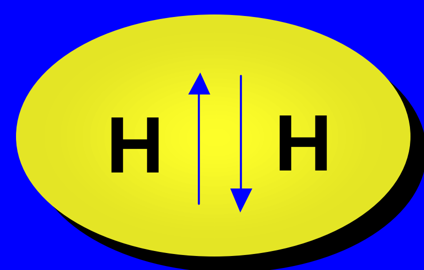

maximum net attraction
(minimum potential energy)
at 74 pm internuclear distance
Potential
energy
74 pm
H• + H•
H-----H
H----H
H---H
-436 kJ/mol
H2
Internuclear distance

Figure 1.14

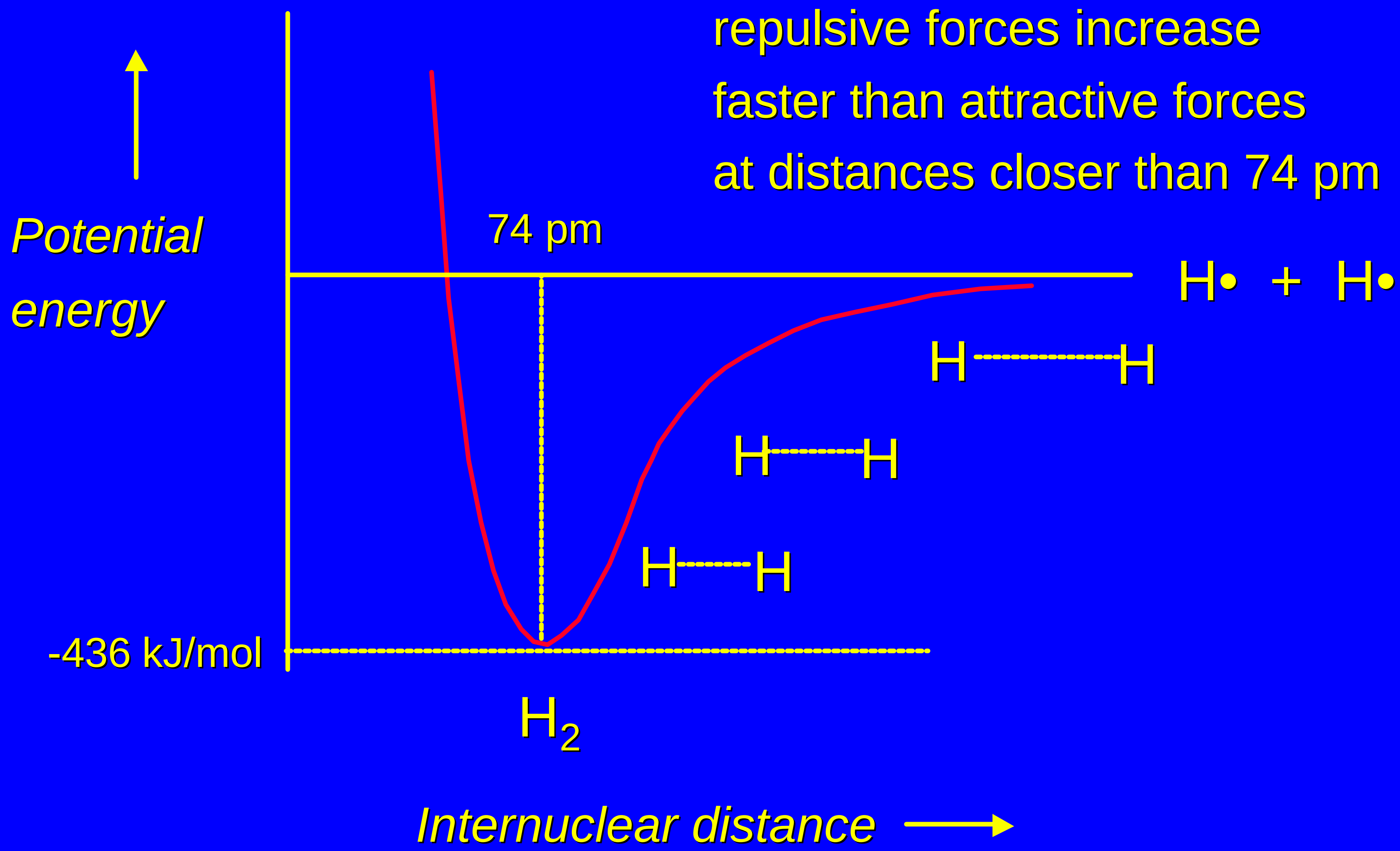


2 H atoms: each electron "feels" attractive force of one proton



H_2 molecule: each electron "feels" attractive force of both protons

Figure 1.14



repulsive forces increase
faster than attractive forces
at distances closer than 74 pm
Potential energy
74 pm
H• + H•
H H
H H
H H
-436 kJ/mol
H2
Internuclear distance

Models for Chemical Bonding

Valence Bond Theory

constructive interference between two electron waves is basis of shared-electron bond

Molecular Orbital Theory

derive wave functions of molecules by combining wave functions of atoms

1.13

Bonding in H_2:

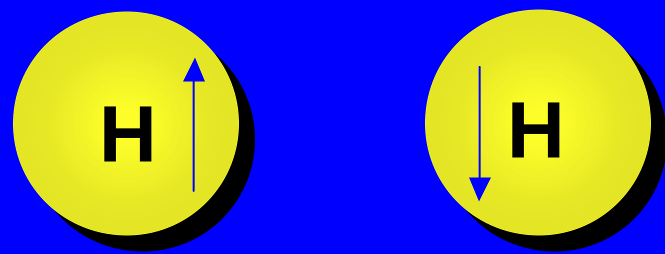
The Valence Bond Model

Valence Bond Model

Electron pair can be shared when half-filled orbital of one atom overlaps in phase with half-filled orbital of another.

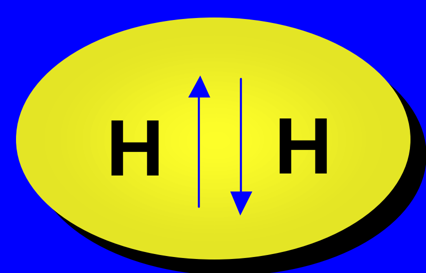
Valence Bond Model

1*s*



1*s*

in-phase overlap of two half-filled hydrogen 1s orbitals

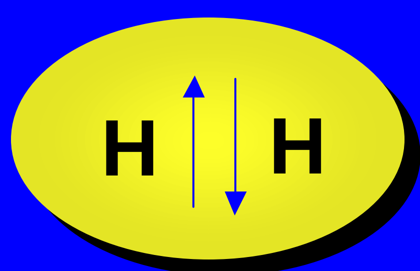


σ bond of H_2

Valence Bond Model

σ Bond: orbitals overlap along internuclear axis

Cross section of orbital perpendicular to internuclear axis is a circle.



Valence Bond Model of H_2

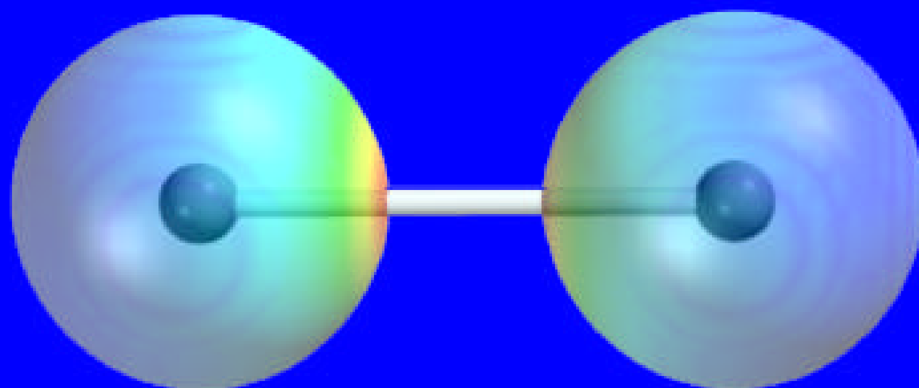


Figure 1.17(*a*) The 1*s* orbitals of two separated hydrogen atoms are far apart. Essentially no interaction. Each electron is associated with a single proton.

Valence Bond Model of H_2

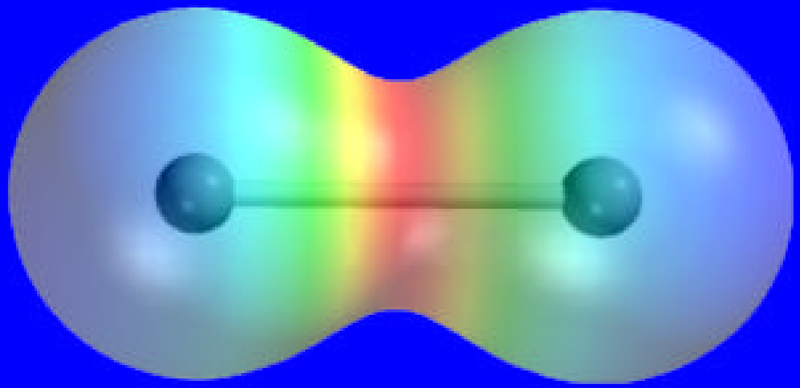


Figure 1.17(*b*) As the hydrogen atoms approach each other, their 1*s* orbitals begin to overlap and each electron begins to feel the attractive force of both protons.

Valence Bond Model of H_2

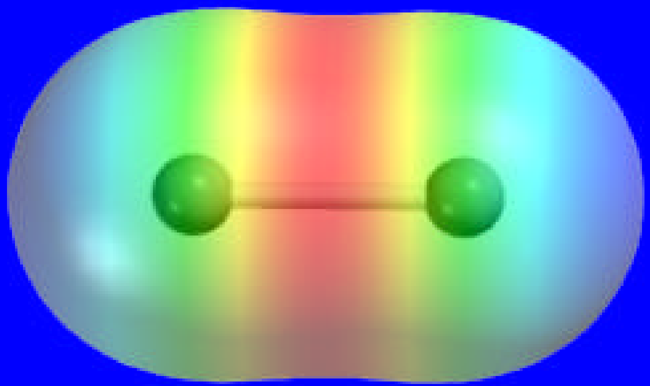


Figure 1.17(*c*) The hydrogen atoms are close enough so that appreciable overlap of the the two 1*s* orbitals occurs. The concentration of electron density in the region between the two protons is more readily apparent.

Valence Bond Model of H_2

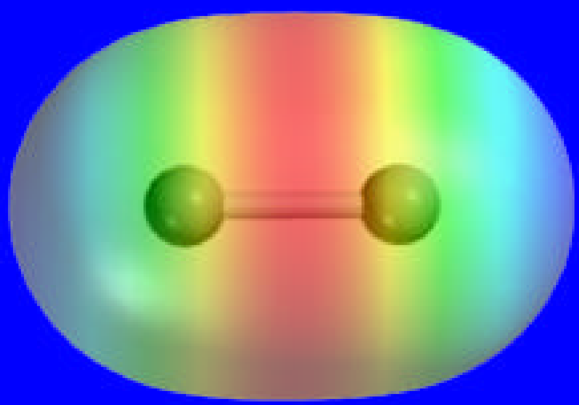


Figure 1.17(*d*) A molecule of H_2. The two hydrogen 1*s* orbitals have been replaced by a new orbital that encompasses both hydrogens and contains both electrons.

1.14

Bonding in H_2:

The Molecular Orbital Model

Main Ideas

Electrons in a molecule occupy molecular orbitals (MOs) just as electrons in an atom occupy atomic orbitals (AOs).

Two electrons per MO, just as two electrons per AO.

Express MOs as combinations of AOs.

MO Picture of Bonding in H_2

Linear combination of atomic orbitals method expresses wave functions of molecular orbitals as sums and differences of wave functions of atomic orbitals.

Two AOs yield two MOs

Bonding combination

$\psi_{MO} = \psi(H)_{1s} + \psi(H')_{1s}$

Antibonding combination

$\psi'_{MO} = \psi(H)_{1s} - \psi(H')_{1s}$

Fig. 1.19: Energy-Level Diagram for H_2 MOs

1*s* —— —— 1*s*

AO AO

Fig. 1.19: Energy-Level Diagram for H_2 MOs

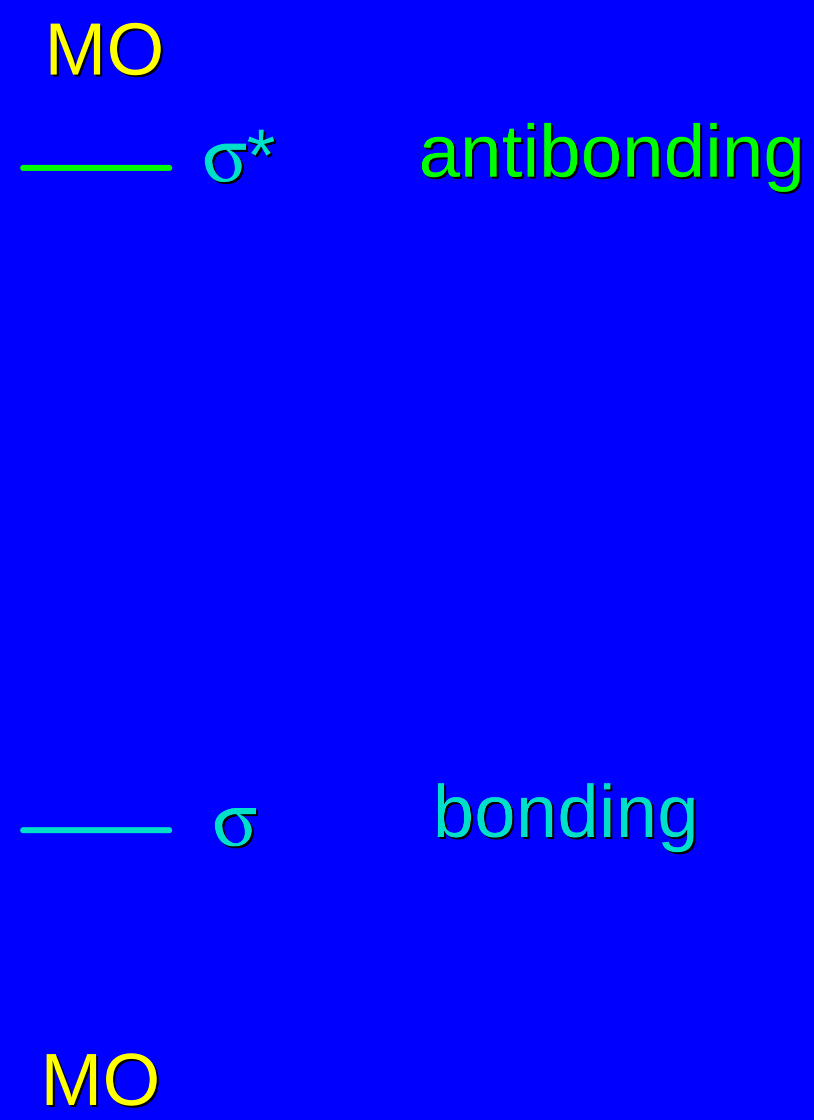


Fig. 1.19: Energy-Level Diagram for H_2 MOs

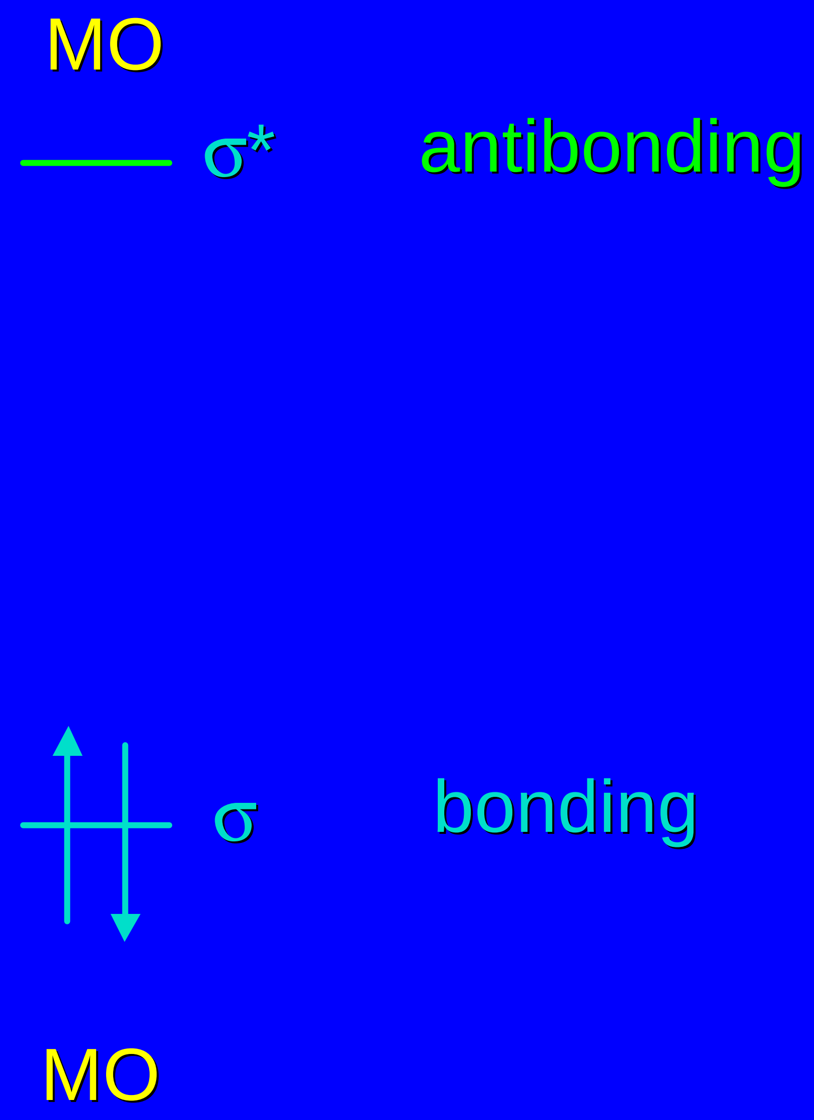


Fig. 1.19: Energy-Level Diagram for H_2 MOs