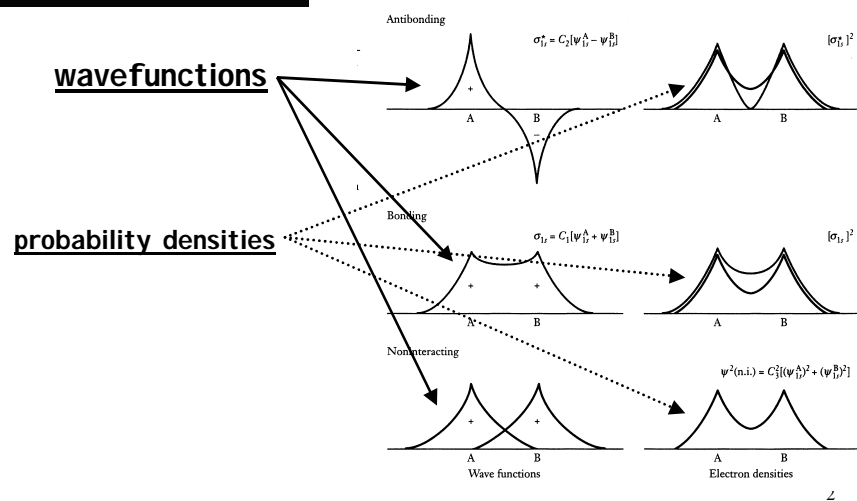


# Announcements – 11/8/00

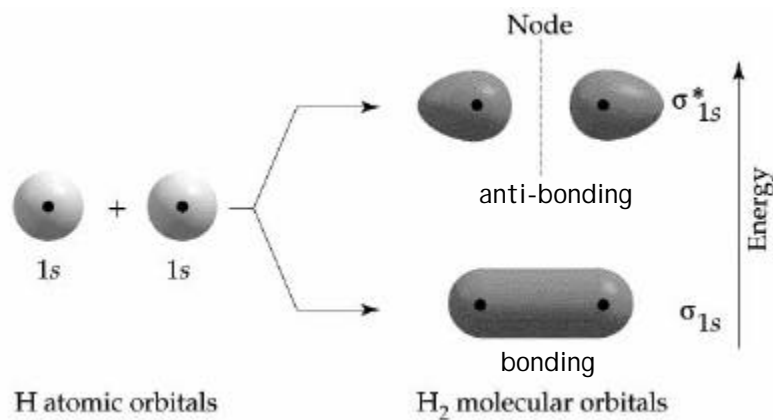
- **Exam #3** - Wed., 11/15/00, 7pm
  - Info page on website
  - Covers material through this Friday
  - See me ASAP if you have a time conflict
  
- **Quiz this Friday!**

1

# Hydrogen Wavefunctions



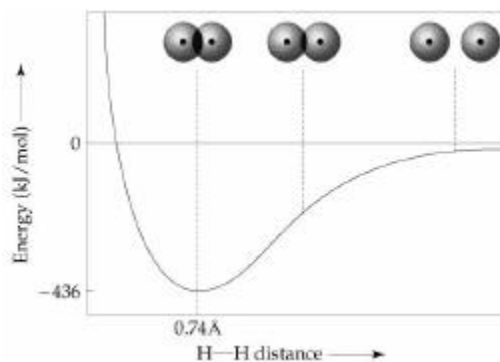
# Hydrogen Molecular Orbitals



3

# Hydrogen MO Formation: Internuclear Separation

- SWE solved with nuclei *at a specific separation distance* . . . How does the **energy** of the new MO vary with **internuclear separation**?



movie

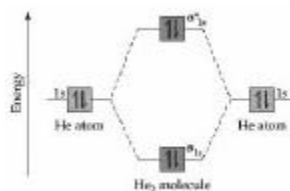
4

# MO Theory: Homonuclear Diatomic Molecules

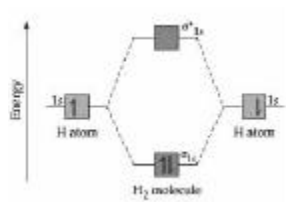
- Let's look at the *s*-bonding properties of some homonuclear diatomic molecules:

**Bond order =**

$$\frac{1}{2}(\text{bonding } e^- - \text{anti-bonding } e^-)$$



**For He<sub>2</sub>:** B.O. = 1 - 1 = 0  
(no bond)



**For H<sub>2</sub>:** B.O. = 1 - 0 = 1  
(single bond)

5

## Configurations and Bond Orders: 1st Period Diatomics

<u>Species</u>	<u>Config.</u>	<u>B.O.</u>	<u>Energy</u>	<u>Length</u>
H <sub>2</sub> <sup>+</sup>	(σ <sub>1s</sub> ) <sup>1</sup>	½	255 kJ/mol	1.06 Å
H <sub>2</sub>	(σ <sub>1s</sub> ) <sup>2</sup>	1	431 kJ/mol	0.74 Å
He <sub>2</sub> <sup>+</sup>	(σ <sub>1s</sub> ) <sup>2</sup> (σ* <sub>1s</sub> ) <sup>1</sup>	½	251 kJ/mol	1.08 Å
He <sub>2</sub>	(σ <sub>1s</sub> ) <sup>2</sup> (σ* <sub>1s</sub> ) <sup>2</sup>	0	~0	LARGE

6

## Combining p-orbitals: $\sigma$ and $\pi$ MO's

