

LECTURE 14 MOLECULAR ORBITAL THEORY

I. Linear combination of atomic orbitals (LCAO)

- A. Molecular orbitals (MOs)
- B. Bonding orbital
- C. Antibonding orbital
- D. Electron configurations
 - 1. Example 1: H_2
 - 2. Example 2: He_2
- E. Bond Order

II. MOs formed by LCAO

- A. MOs formed by LCAO – 2s
 - 1. Example 1: Li_2
 - 2. Example 2: Be_2
- B. Bonding MOs formed by LCAO – $2p_x$ and $2p_y$
 - 1. Example 1: B_2
 - 2. Example 2: C_2
- C. Bonding MO formed by LCAO – $2p_z$
- D. Antibonding MO formed by LCAO – $2p_x$ and $2p_y$
- E. Antibonding MO formed by LCAO – $2p_z$

III. Molecular Orbital Theory: Heteronuclear Diatomics