Reading, etc.

- Continuation of Chapter 3. Sections 3-7 – 3.10 in this set of notes.
- Download the “resume of MO theory” from the class Web site for use in conjunction with today’s class.

Intro to MO Theory

- Usual approach: Linear Combination of Atomic Orbitals:

  \[
  \psi_{\mu} = \sum_{i=1}^{N} c_{\mu i} \varphi_{i}
  \]

  Atomic Orbitals: \( \{ \varphi_{i} ; i = 1, \ldots, N \} \)
  Molecular Orbitals: \( \{ \psi_{\mu} ; \mu = 1, \ldots, N \} \)

- Coefficients give the contributions that each of the individual AOs make to the MO

MO Theory - General Features

Starting with \( N \) AOs, we can make \( N \) molecular orbitals. No more and no less.

MOs are mutually orthogonal and normalized: overlap between any two MOs is zero and overlap of a MO with itself = 1.

Pauli exclusion principle: an MO can accommodate 2 electrons. One is spin-up \( (m_s = +1/2) \), one is spin-down \( (m_s = -1/2) \).

\[ \begin{align*}
  H_2 & : \psi = (1/2)(\varphi_1 + \varphi_2) \\
  \text{Energy} & : \sigma_g \\
  \text{Energy} & : \sigma_u \\
  \text{Energy} & : \sigma_u^* \\
  \text{Energy} & : \sigma_g^*
\end{align*} \]
neglected interactions:

s-p mixing

including effects of s-p mixing:
Fig 3-17
energies relative to $1\pi_u$

HF: polarity in a heteronuclear diatomic

CO: more complications

CO: more complications