Chemical Bonding Theory
An explanation for observed chemical and spectroscopic behavior

Items to explain
1. Polarity of bonds
   • IR spectroscopy
   • NMR chemical shifts
2. Electrochemistry
   • Oxidation and reduction potentials lower with conjugation
3. UV spectroscopy
   • Alkanes don’t absorb well
   • Conjugation increases $\lambda_{\text{max}}$
   • Benzene (178 nm) vs. 2,4-hexadiene (240 nm)

Descriptions of Bonding
• Molecular orbital theory
  – Delocalized electrons
  – More difficult to conceive and present
  – “Hydrogen-like Atomic Orbitals” are used to form Molecular Orbitals
• Valence-bond theory
  – Localized electrons
  – Convenient for presentation
  – “Hybrid Atomic Orbitals” are used to form “independent” Valence Bonds

Atomic Orbitals
Atomic Orbitals

Molecular Orbital Theory: $\text{H}_2$

\[ \text{H} - \text{H} = \text{H} \text{ H} \]

\[ \text{H} + \text{H} = \text{H} \text{ H} \]
Molecular Orbital Theory: Ethene

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Valence-bond Theory: $H_2$

\[ H_2 + H_2 = H-H \]

Pictorial VB Theory: sp Hybrids

\[ \text{Pictorial VB Theory: sp Hybrids} \]

\[ \text{animation} \]

Pictorial VB Theory: $sp^2$ Hybrids

\[ \text{Pictorial VB Theory: sp}^2 \text{ Hybrids} \]

\[ \text{animation} \]
This is the carbon-carbon σ (sigma) bond only.
Pictorial VB Theory: Ethene

- This is the carbon-carbon $\sigma + \pi$ (sigma + pi) bonding combination only

Sigma and pi bonding in ethane, ethylene, and acetylene

- Unhybridized $2e$ orbitals
- The other $\pi$ bond