

Chemical Bonding Theory

An explanation for observed chemical and spectroscopic behavior

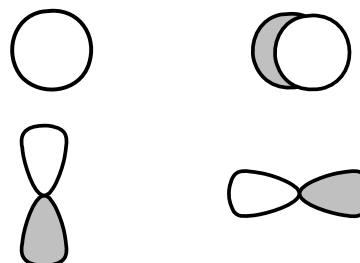
Items to explain

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 λ_{max}
 - Benzene (178 nm) vs. 2,4-hexadiene (240 nm)

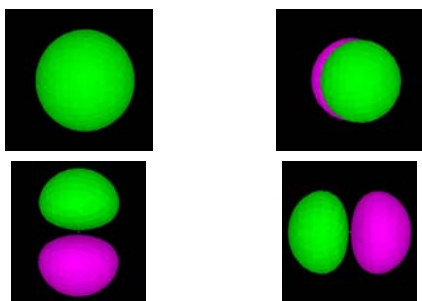
Descriptions of Bonding

- 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

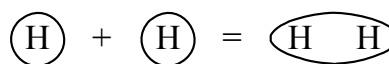
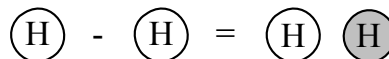
Atomic Orbitals



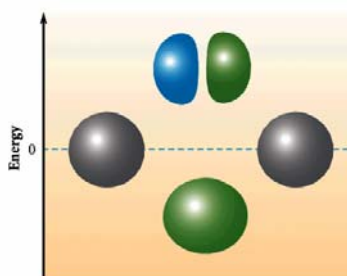
Atomic Orbitals



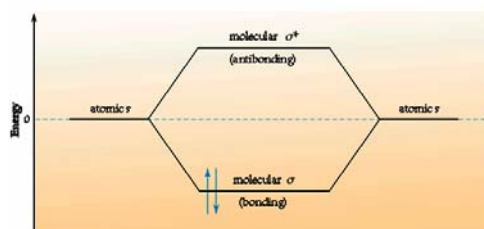
Molecular Orbital Theory: H₂



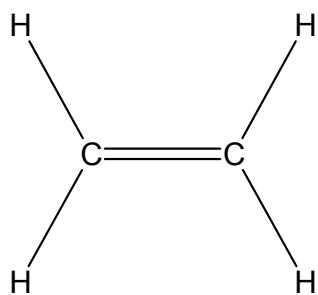
Molecular Orbital Theory: H₂



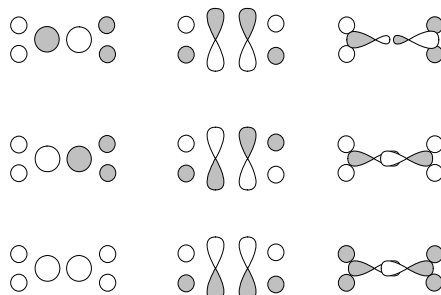
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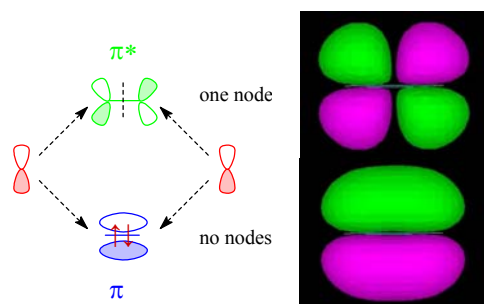
Molecular Orbital Theory: Ethene



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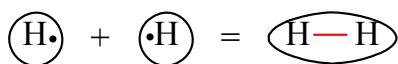
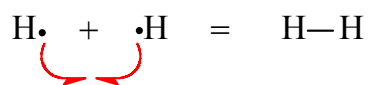
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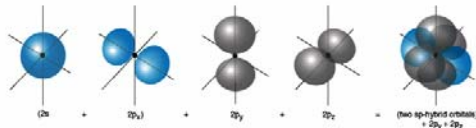
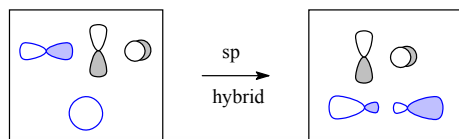
Valence-bond Theory: H₂



Pictorial VB Theory: sp Hybrids

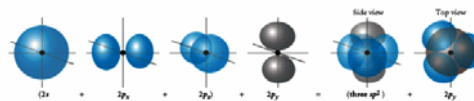
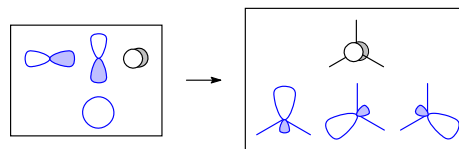


Pictorial VB Theory: sp Hybrids



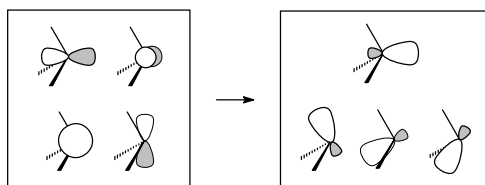
[animation](#)

Pictorial VB Theory: sp² Hybrids



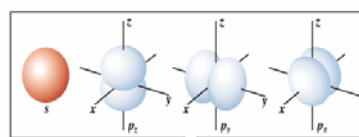
[animation](#)

Pictorial VB Theory: sp^3 Hybrids

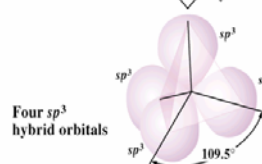


[animation](#)

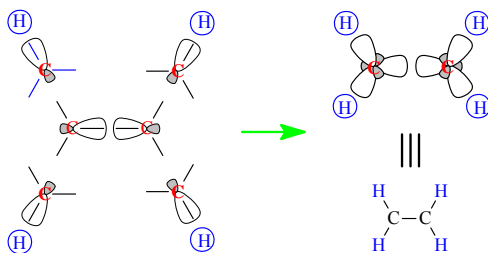
Pictorial VB Theory: sp^3 Hybrids



[animation](#)



Pictorial VB Theory: Ethene

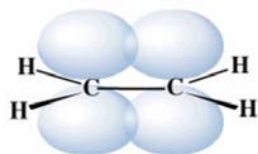


Pictorial VB Theory: Ethene

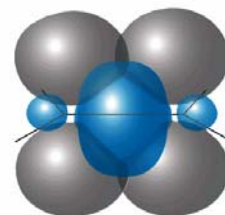


- This is the carbon-carbon σ (sigma) bond **only**

Pictorial VB Theory: Ethene

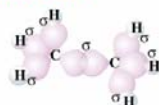


Pictorial VB Theory: Ethene

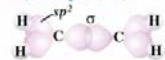


- This is the carbon-carbon $\sigma + \pi$ (sigma + pi) bonding combination **only**

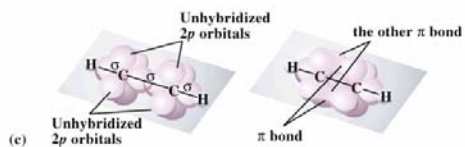
Sigma and pi bonding in ethane, ethylene, and acetylene



(a)



(b)



(c)