Chemical Bonding Theory

An explanation for observed chemical and spectroscopic behavior

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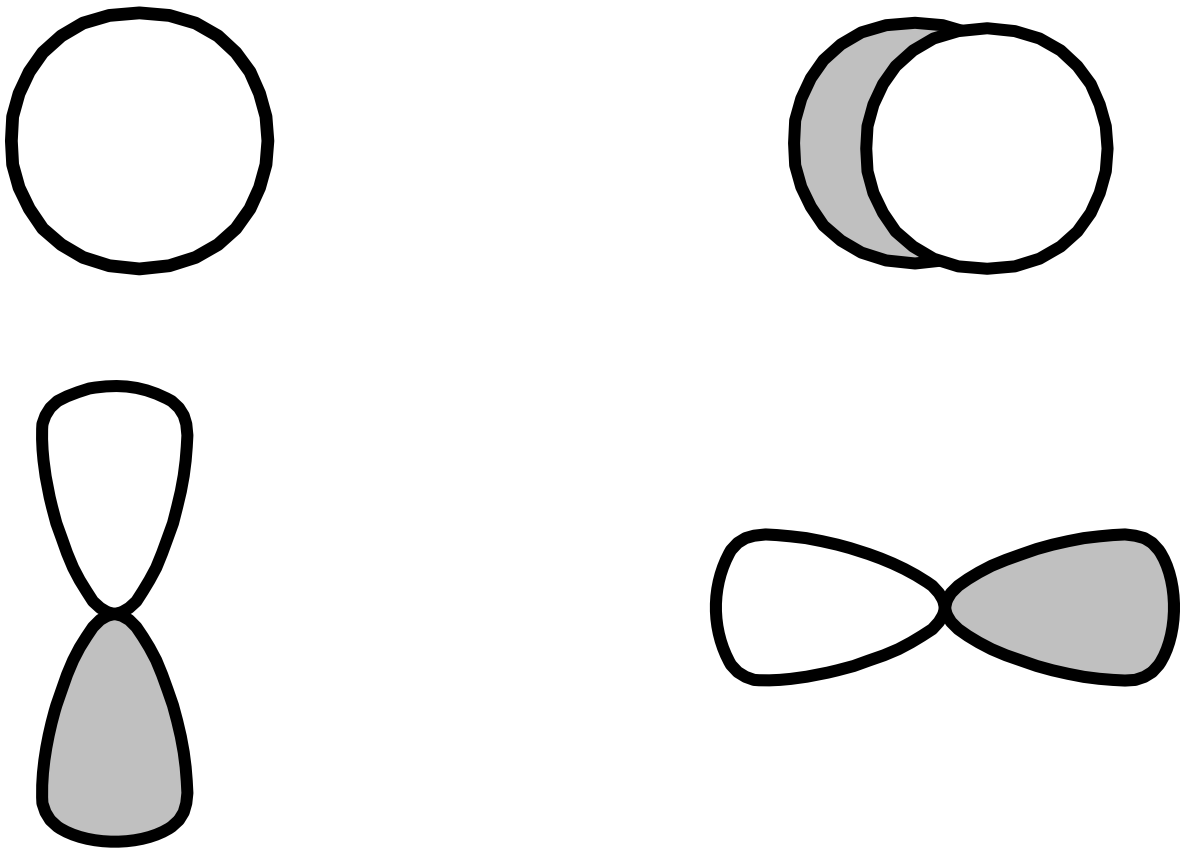
Items to explain

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



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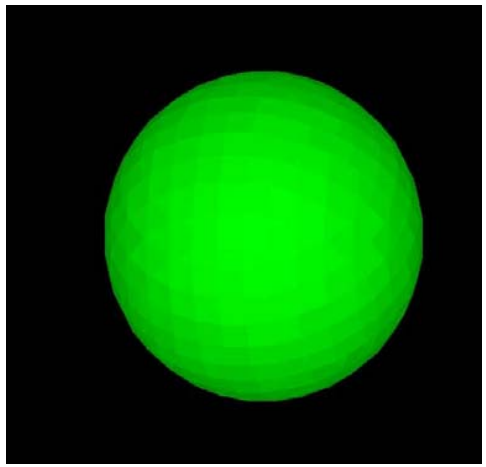
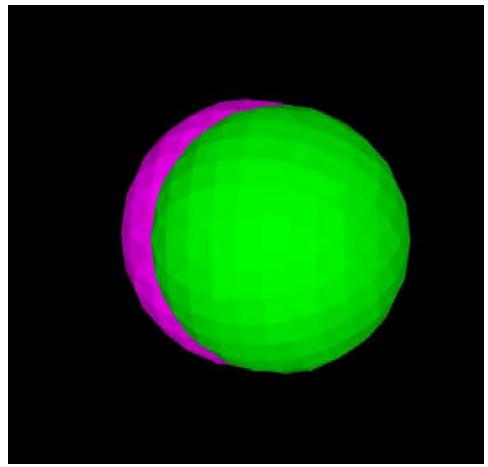
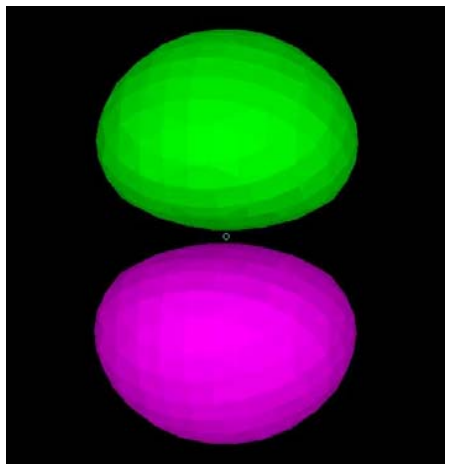
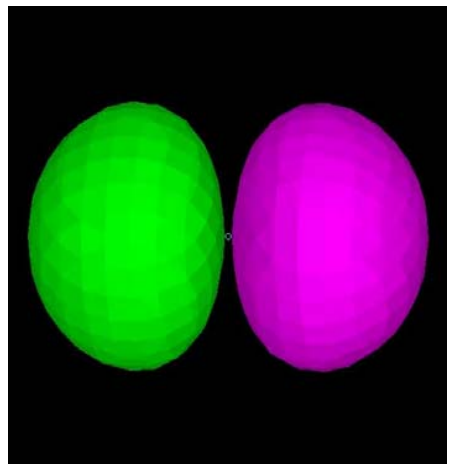
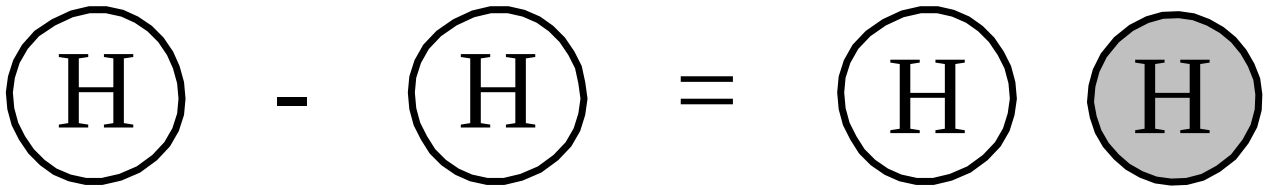


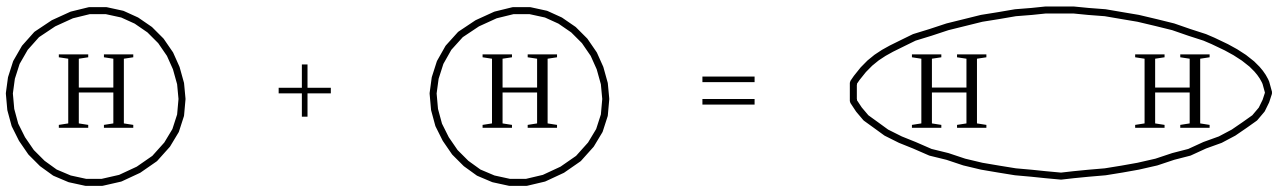






Molecular Orbital Theory: H_2





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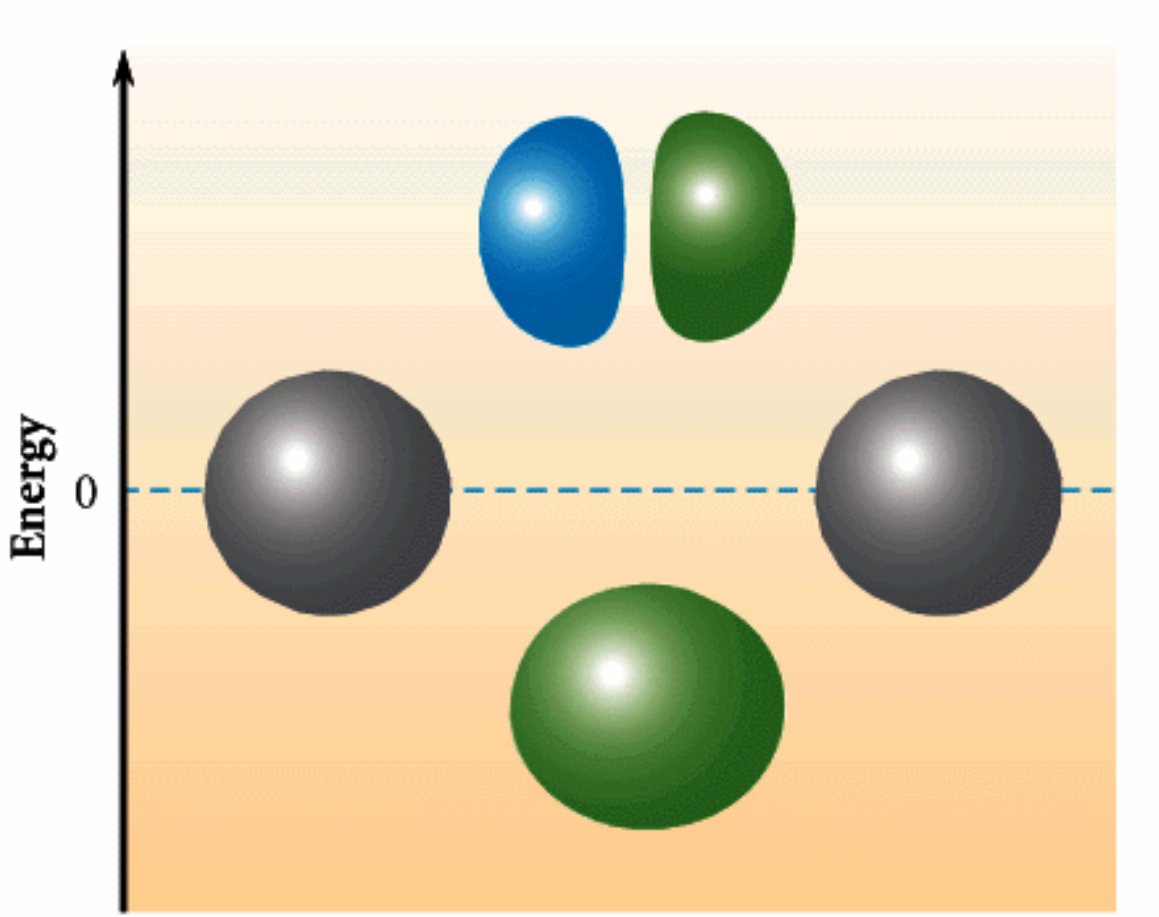

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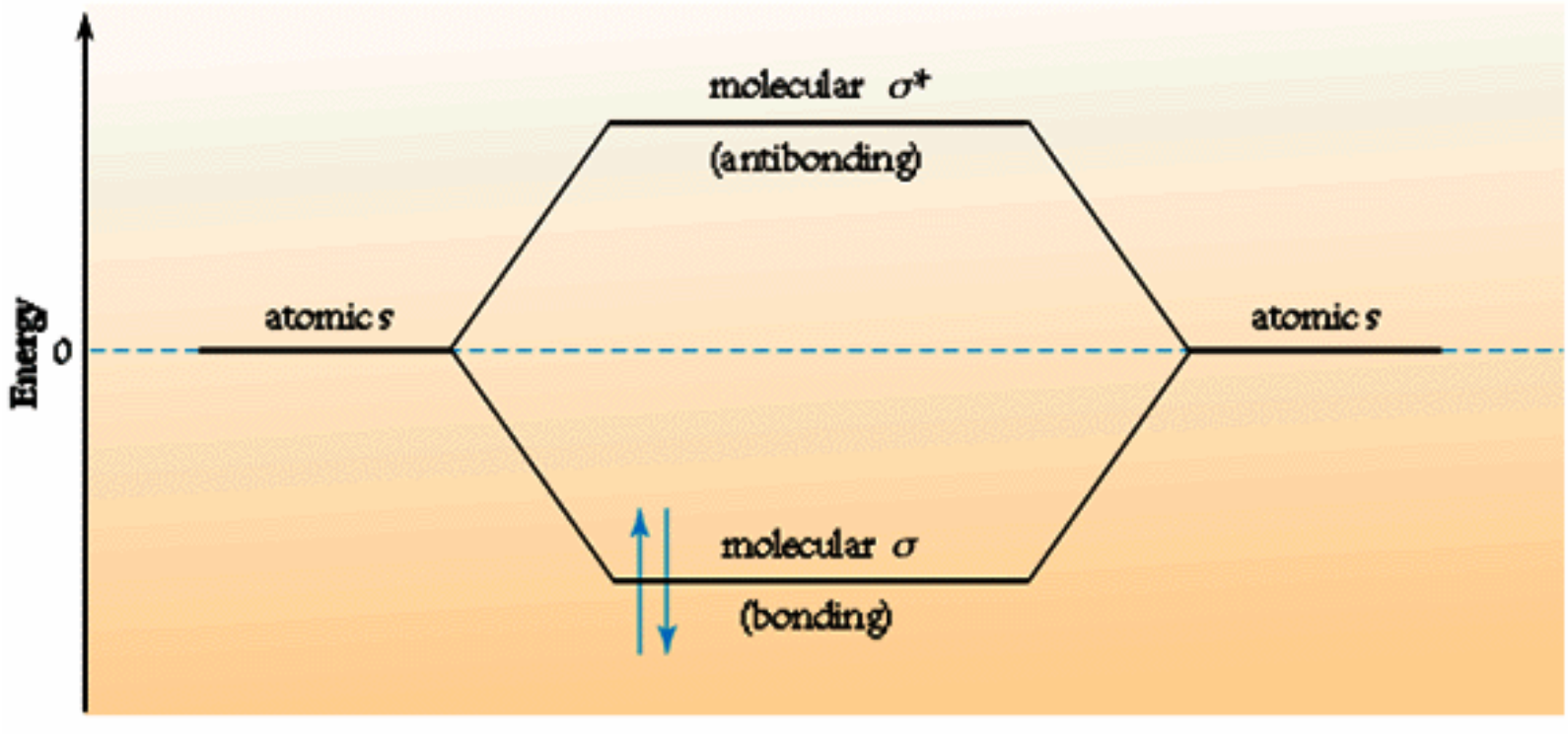
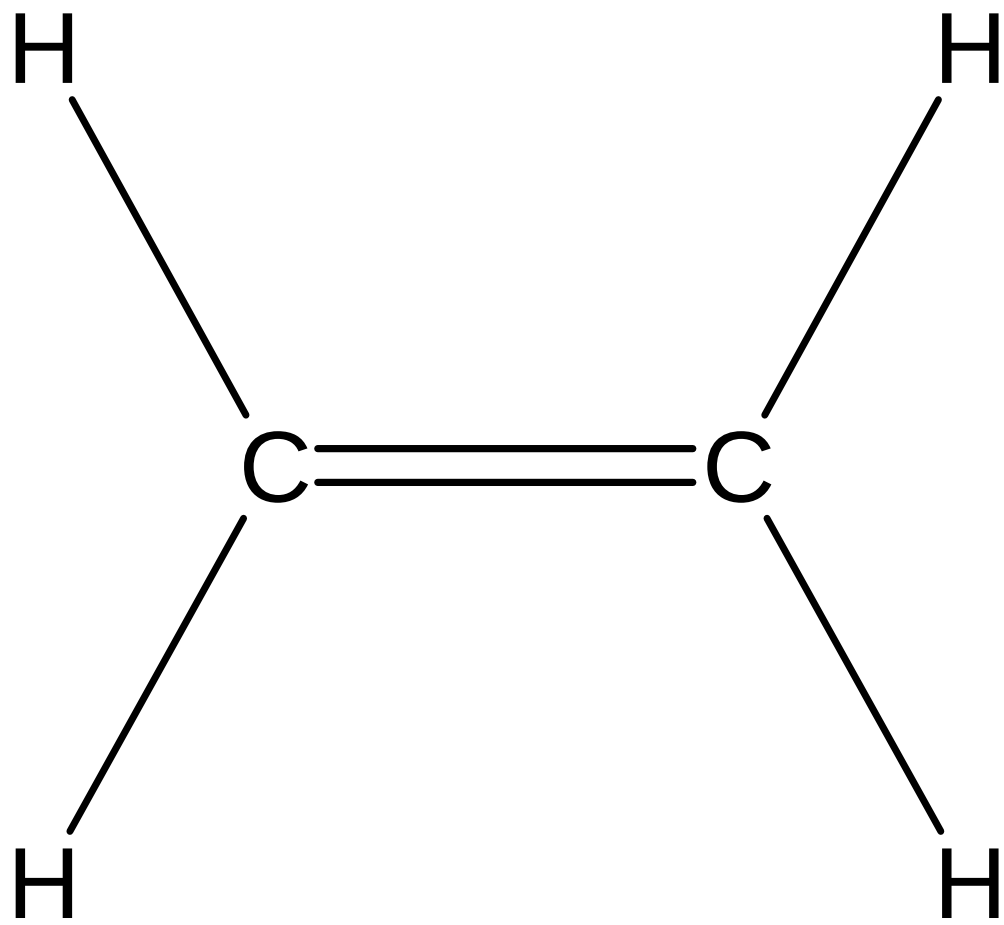


Molecular Orbital Theory: Ethene



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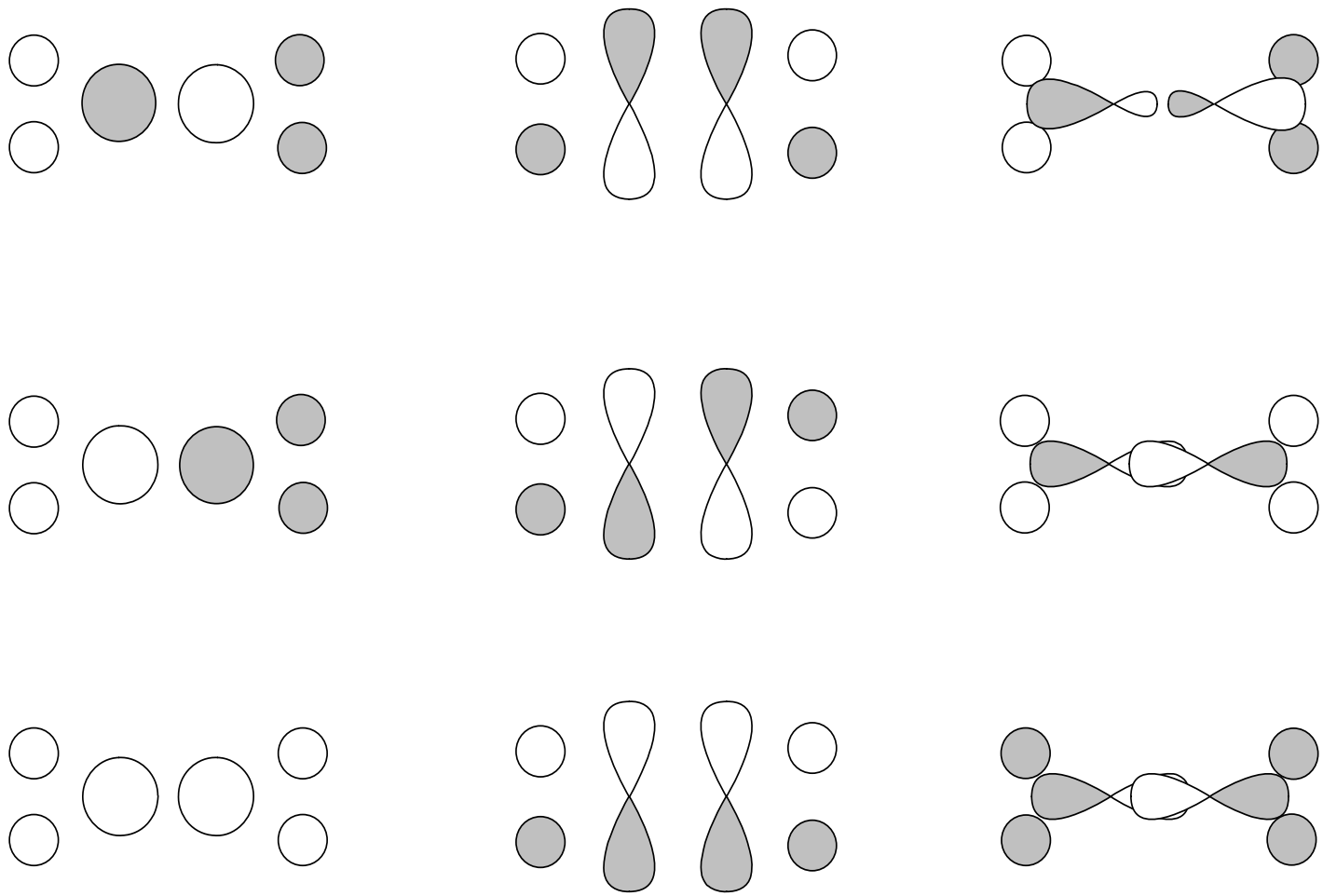

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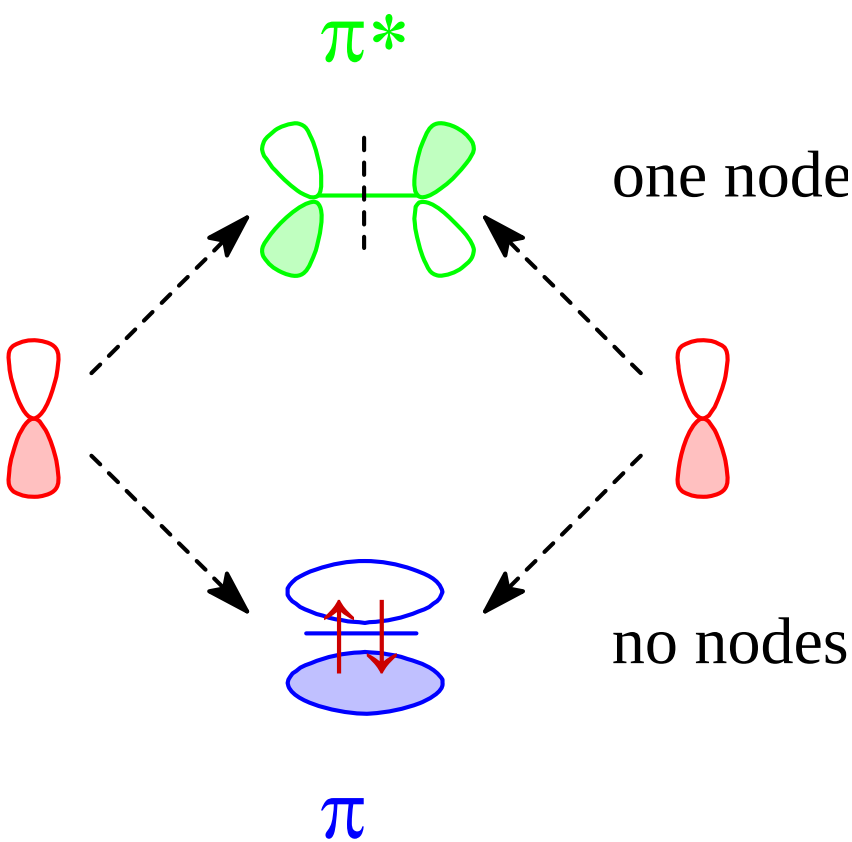

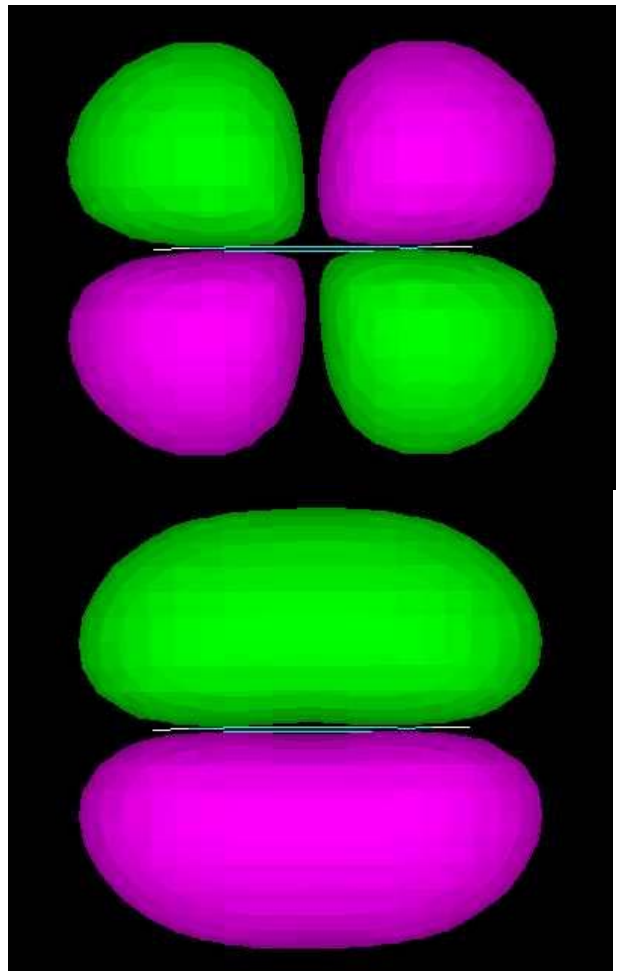

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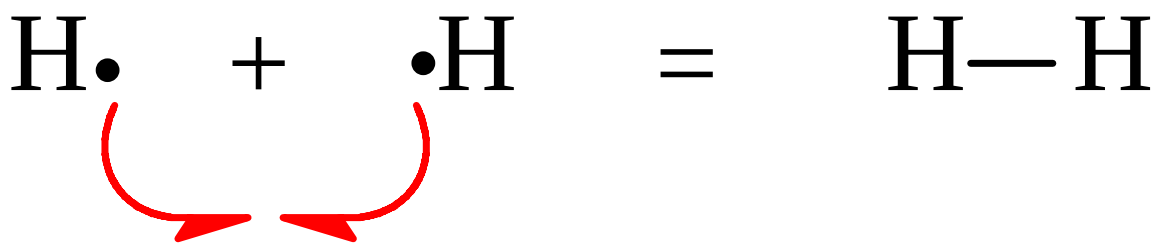
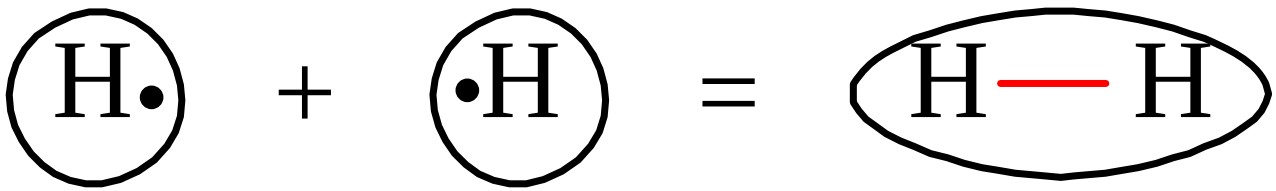
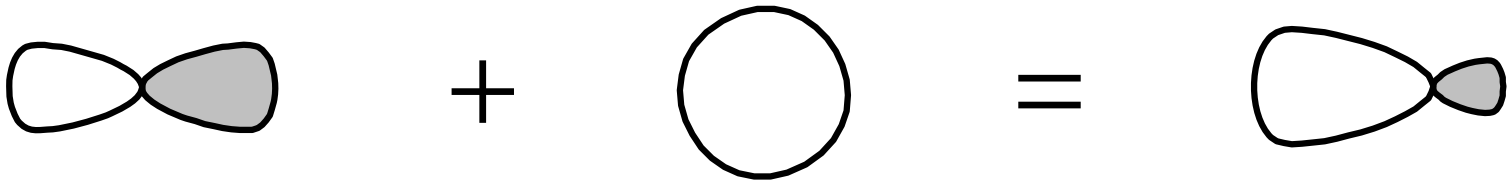
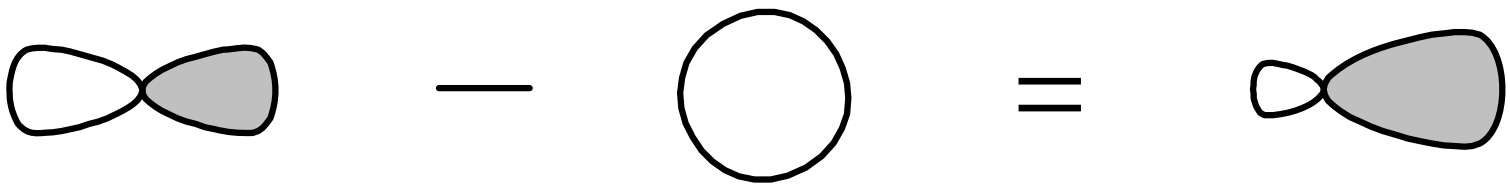
Valence-bond Theory: H_2





Pictorial VB Theory: sp Hybrids





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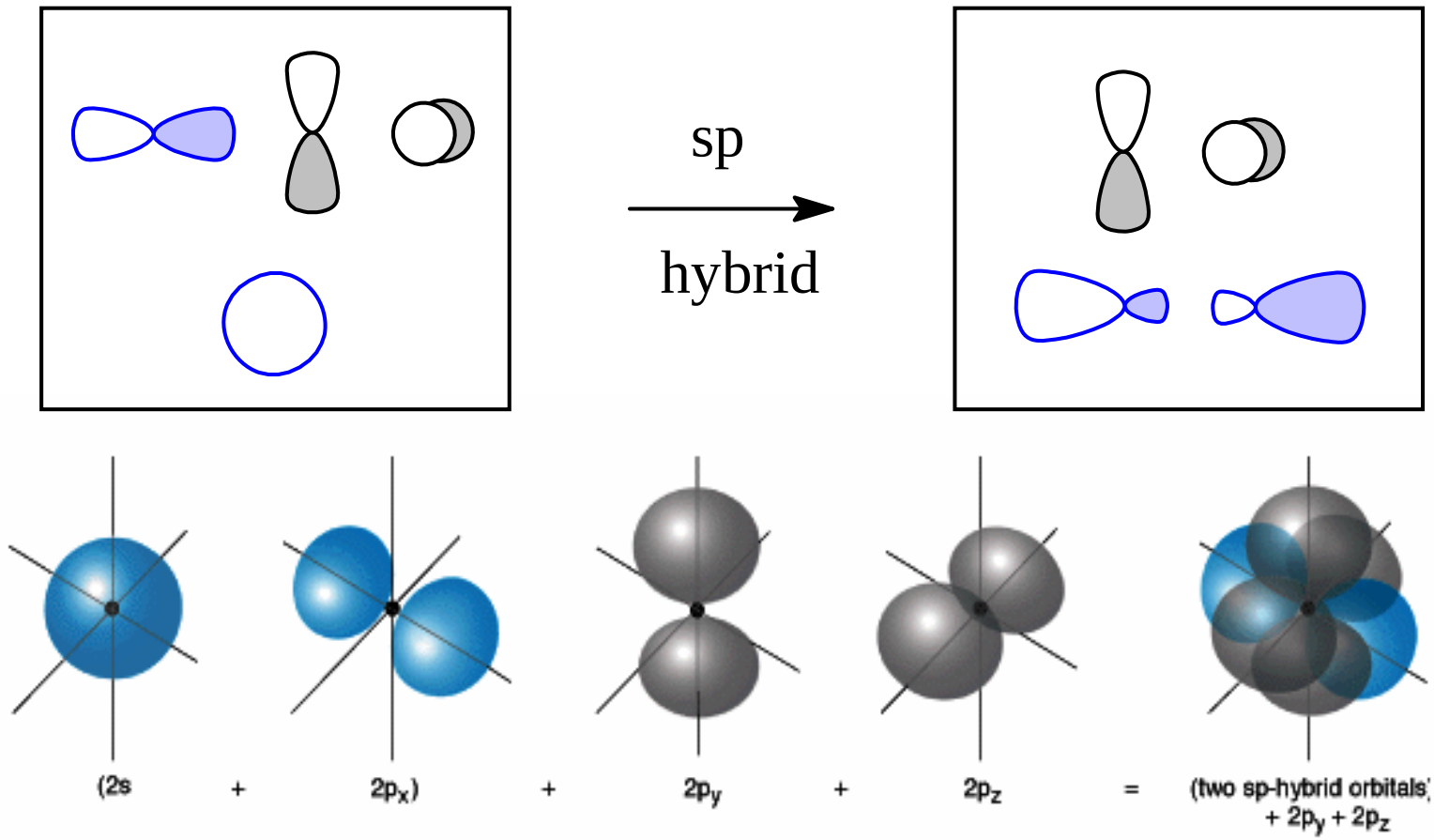

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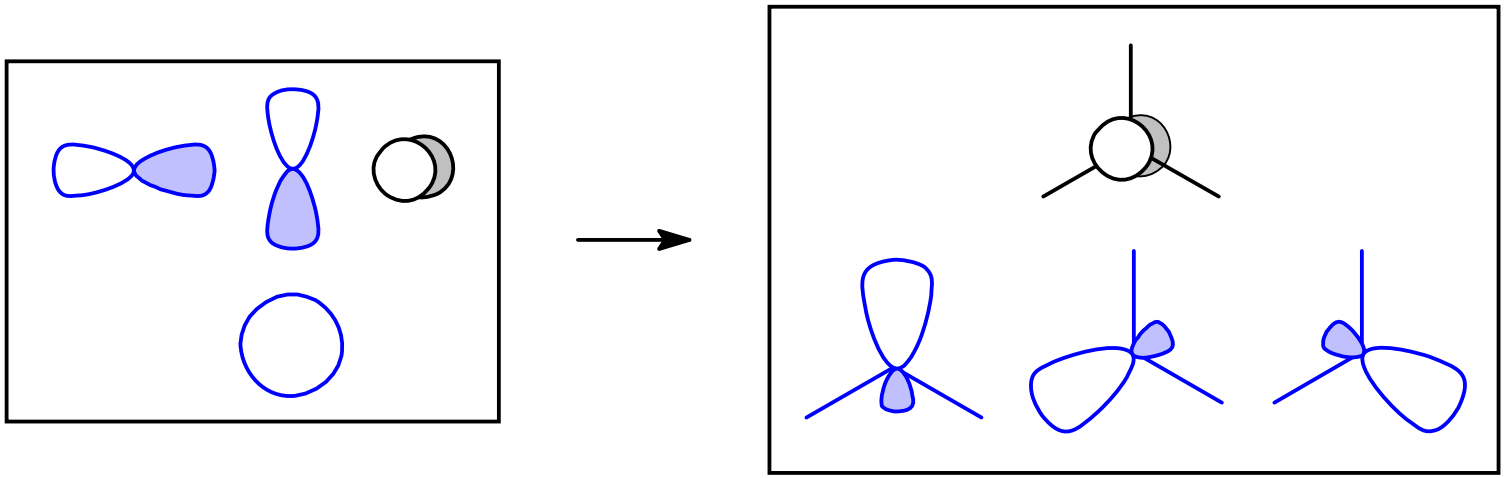
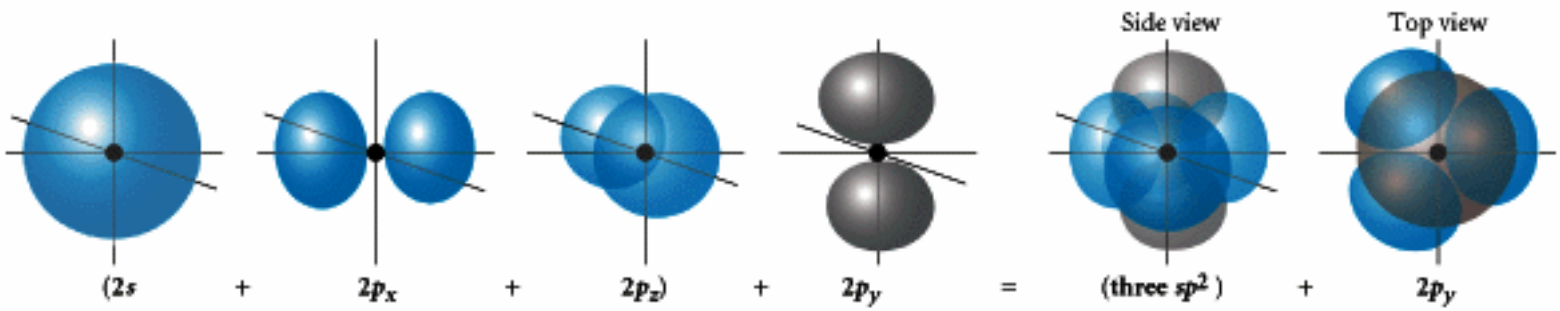
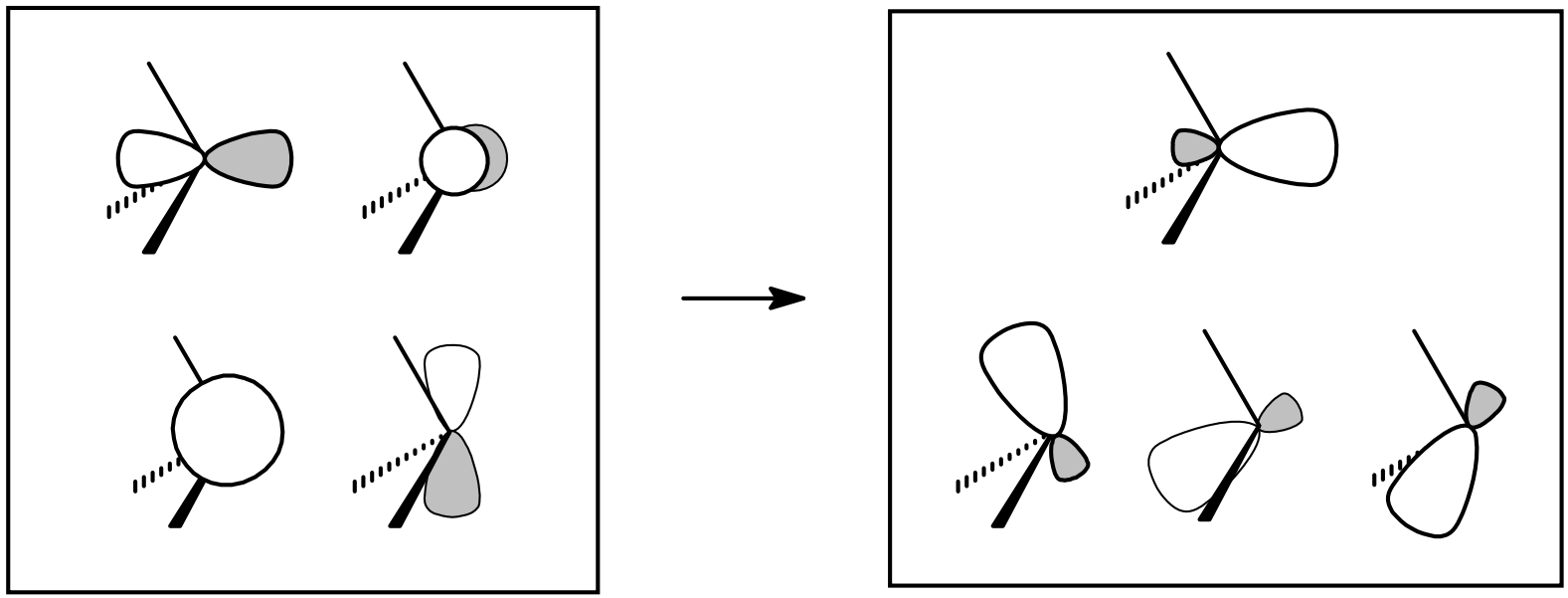
Pictorial VB Theory: sp^2 Hybrids





animation

Pictorial VB Theory: sp^3 Hybrids



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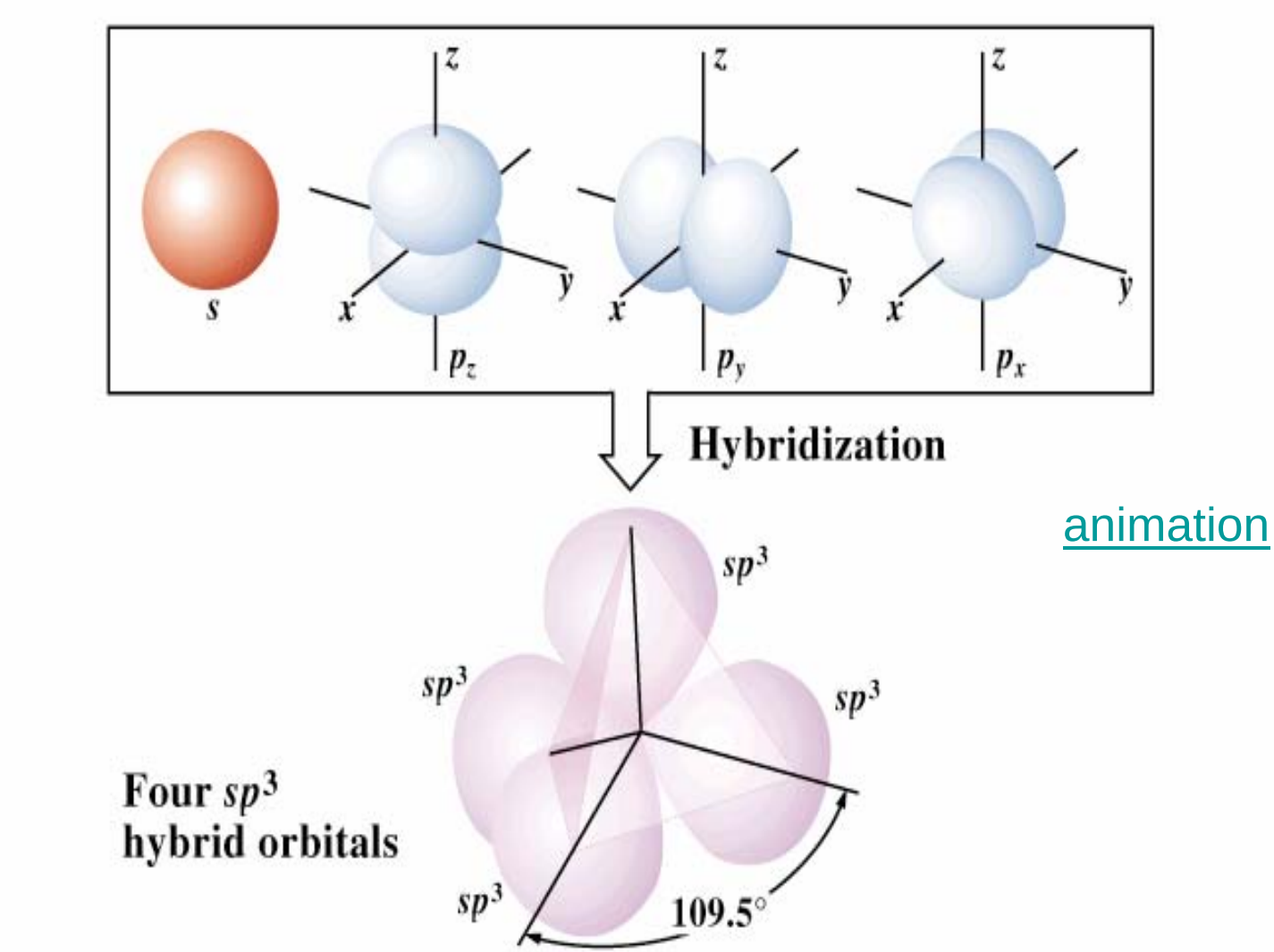
Pictorial VB Theory: sp^3 Hybrids



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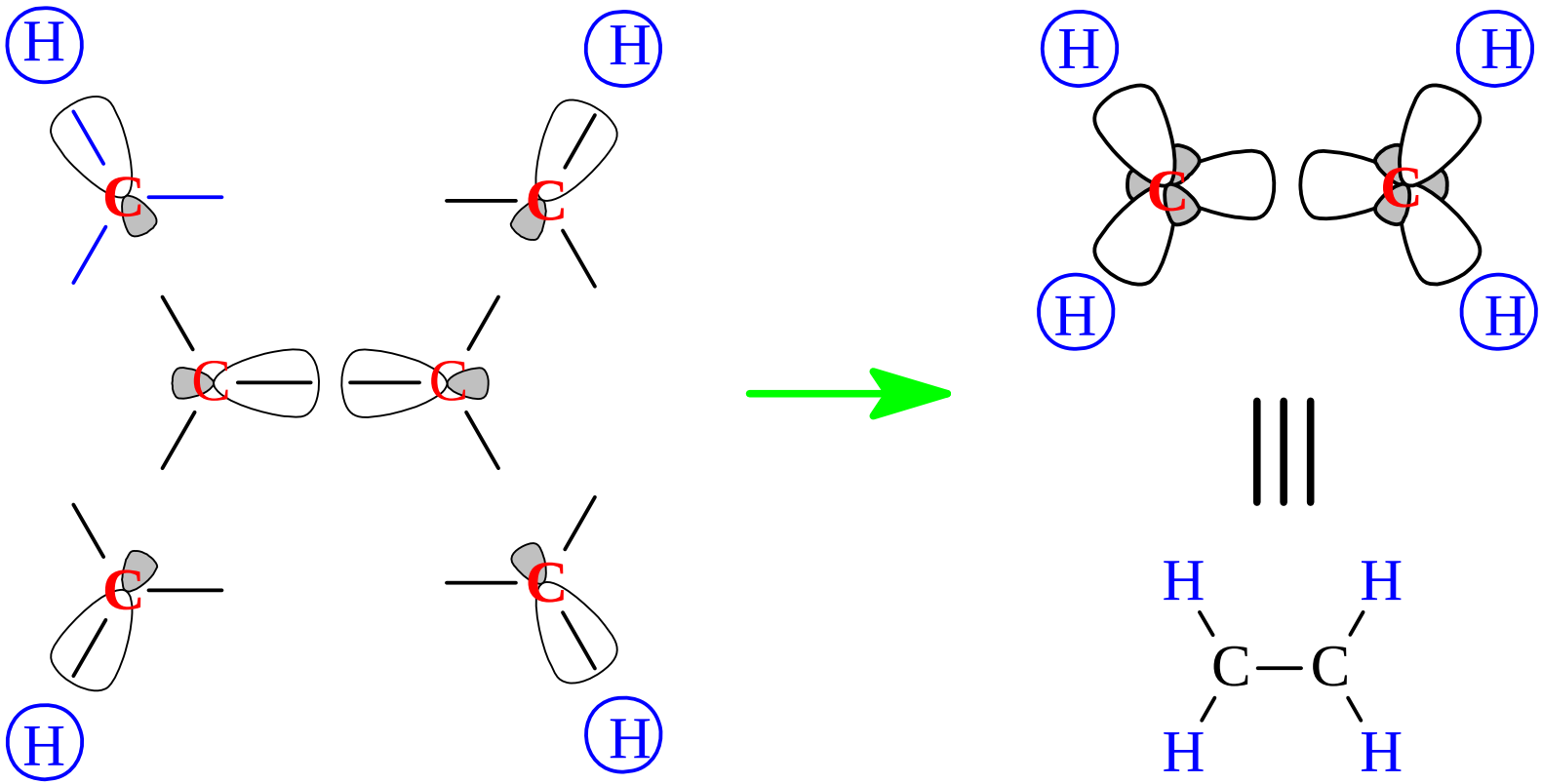
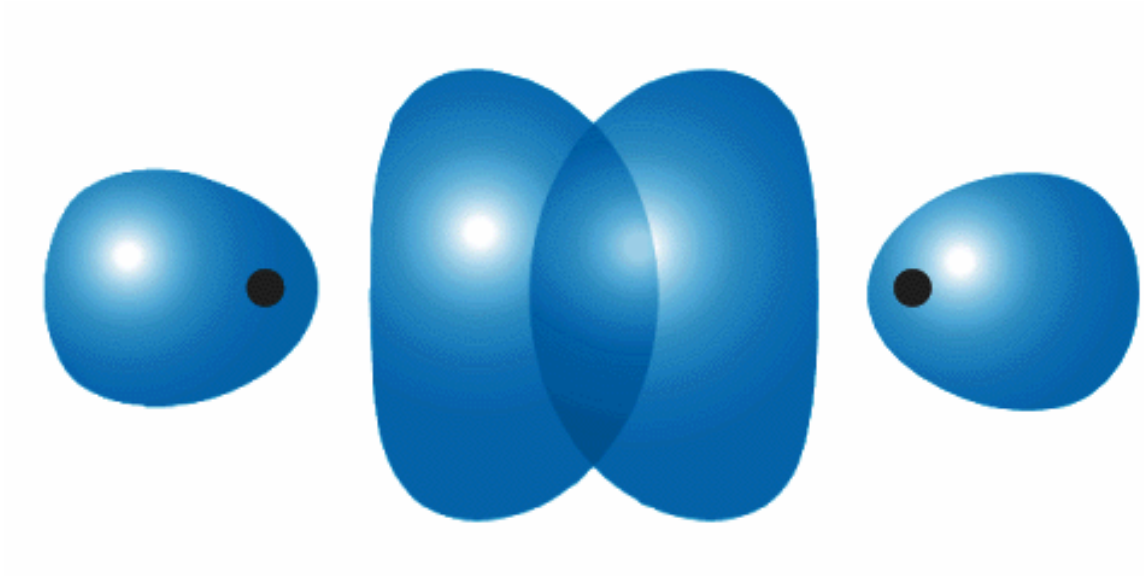
Pictorial VB Theory: Ethene

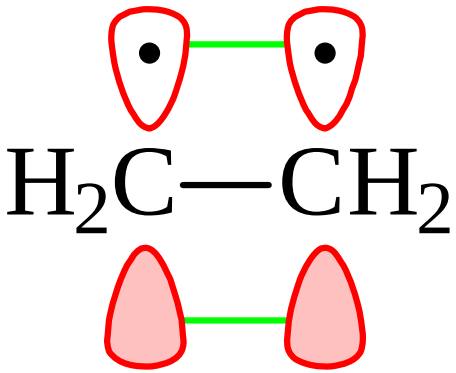


Pictorial VB Theory: Ethene



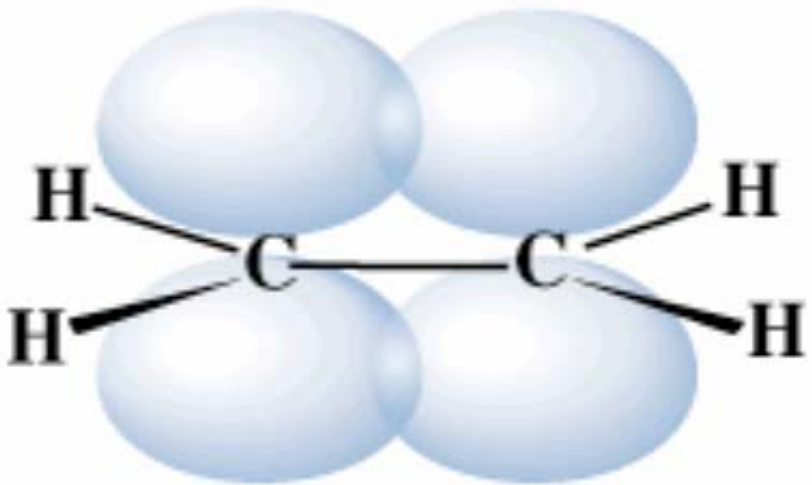
- This is the carbon-carbon σ (sigma) bond **only**

Pictorial VB Theory: Ethene



≡

$H_2C{=}CH_2$



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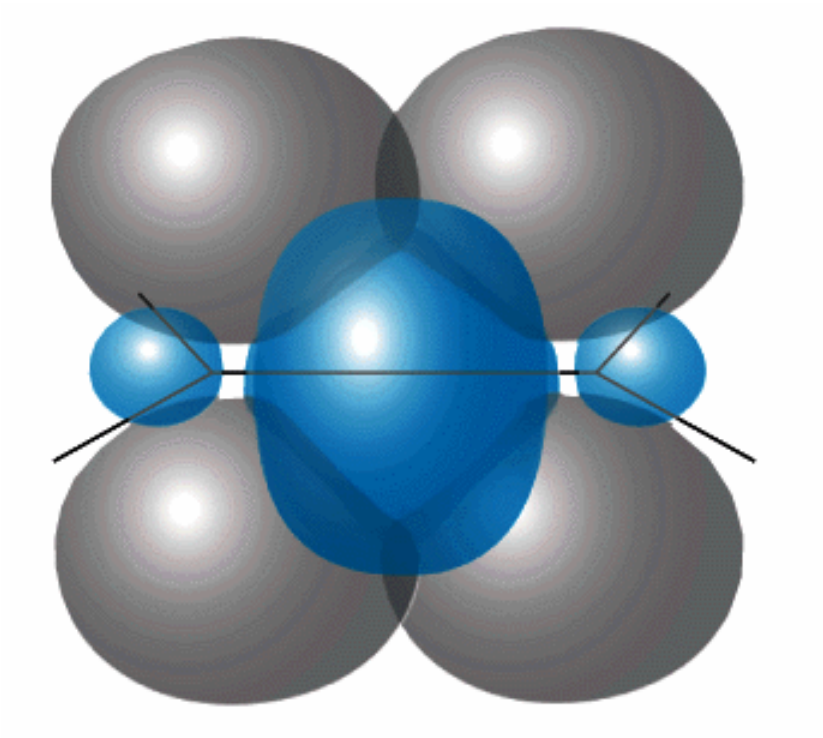
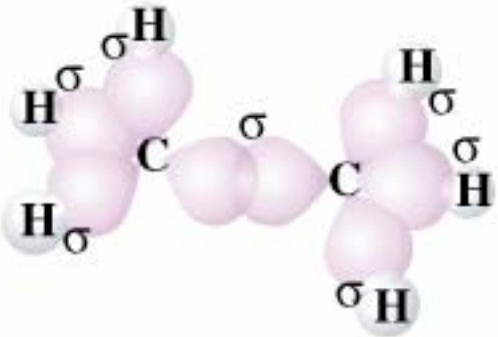
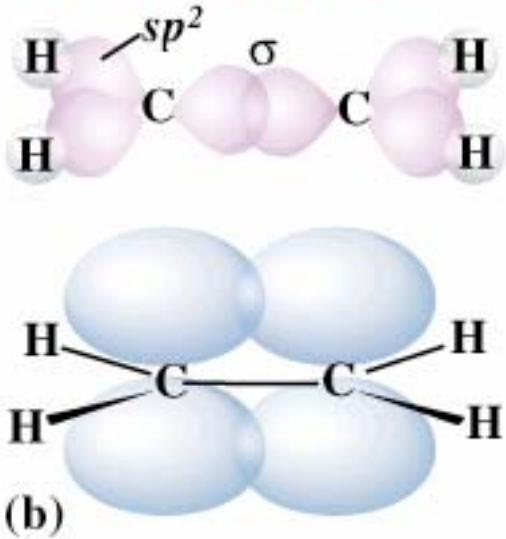


- This is the carbon-carbon σ + π (sigma + pi) bonding combination **only**

Sigma and pi bonding in ethane, ethylene, and acetylene



(a)



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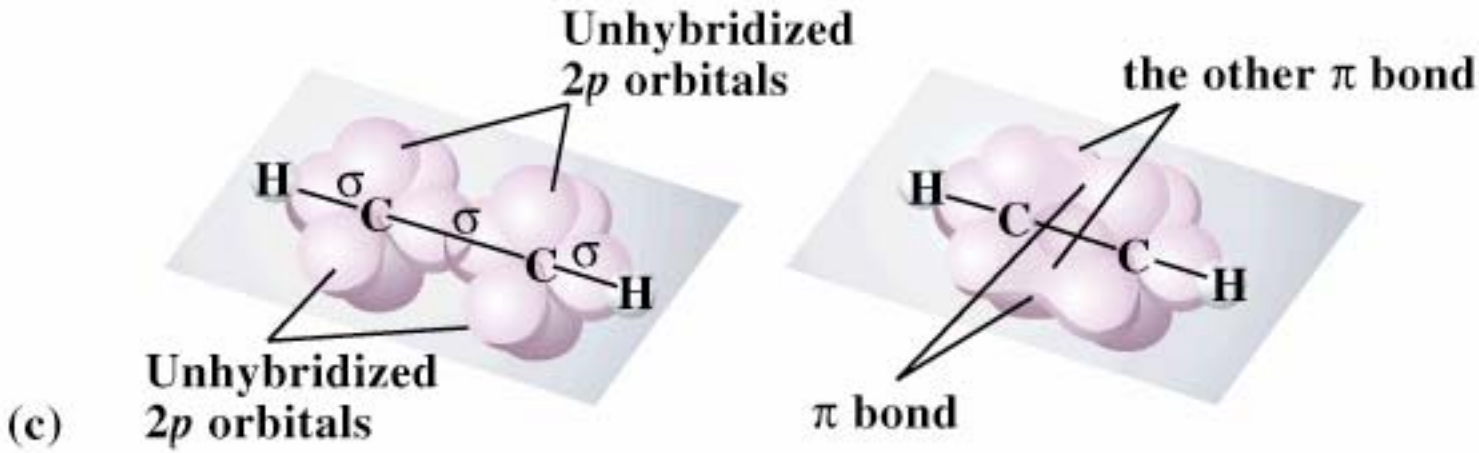

(c)