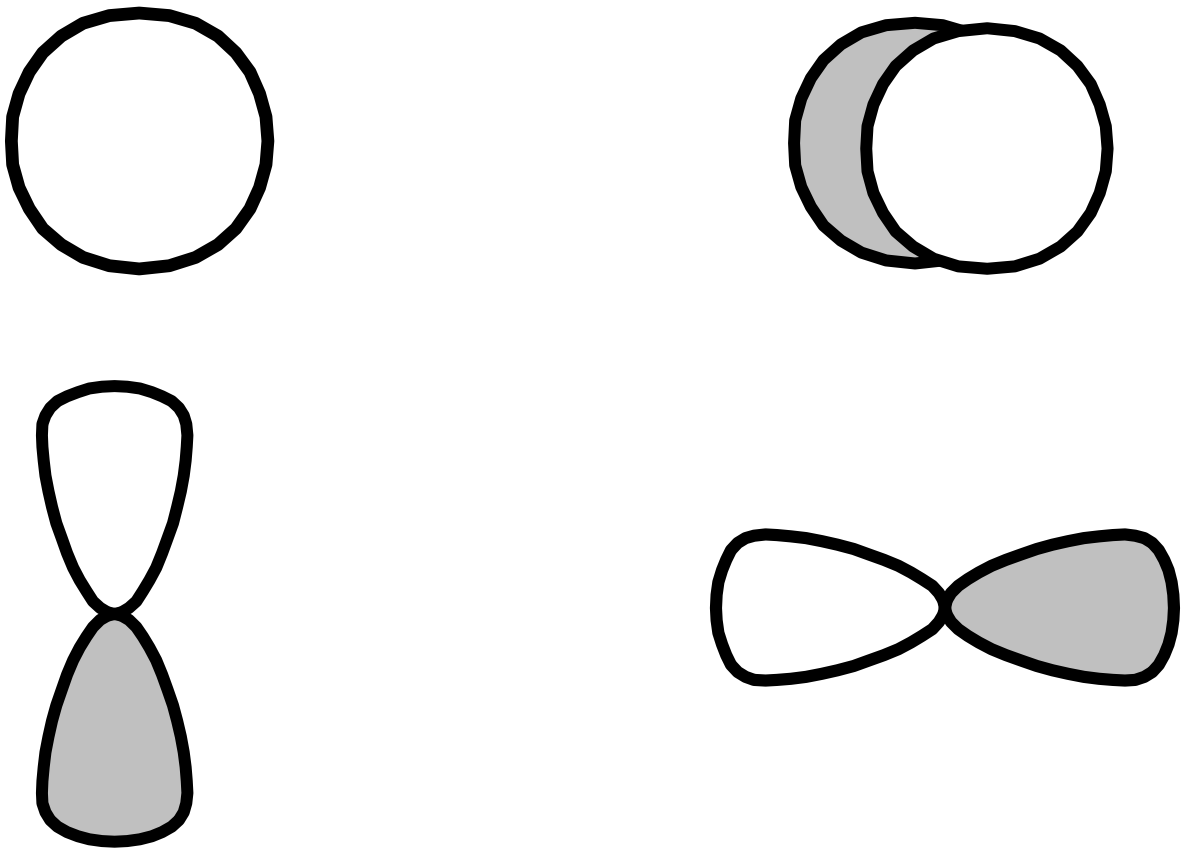
Chemical Bonding Theory

An explanation for observed chemical and spectroscopic behavior

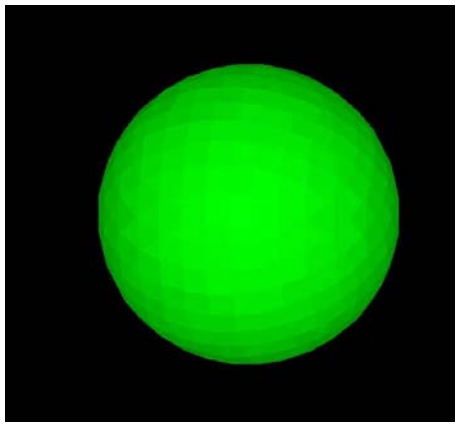
Descriptions of Bonding

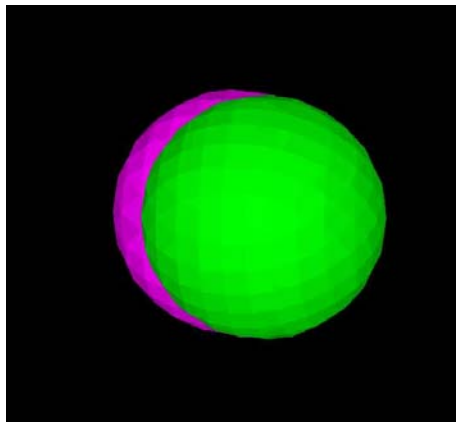
- Valence-bond theory
  - Localized electrons
  - Convenient for presentation
  - “Hybrid Atomic Orbitals” are used to form “independent” Valence Bonds
- Molecular orbital theory
  - Delocalized electrons
  - More difficult to conceive and present
  - “Hydrogen-like Atomic Orbitals” are used to form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

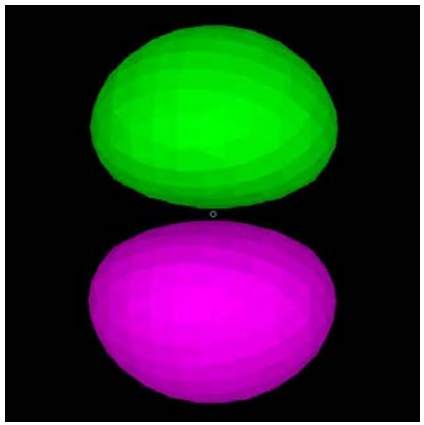
Atomic Orbitals

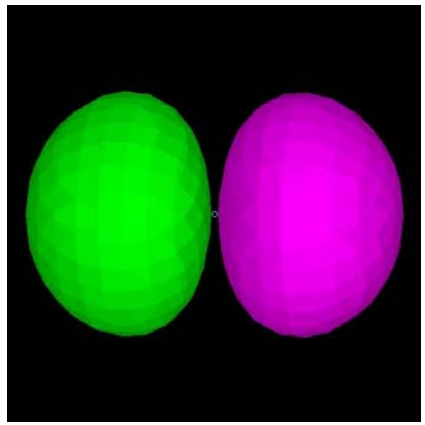


Atomic Orbitals

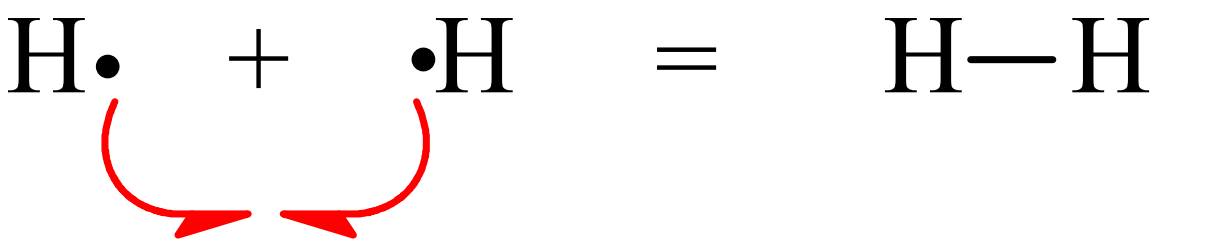


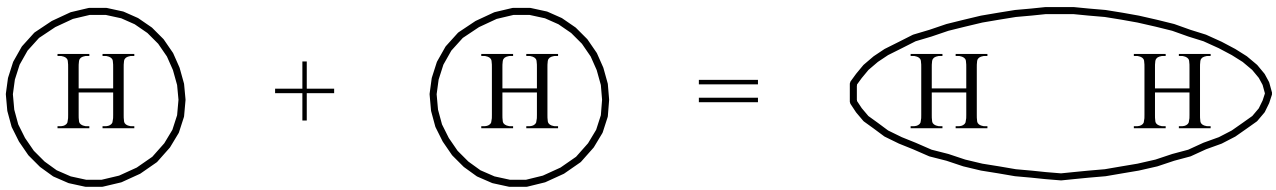




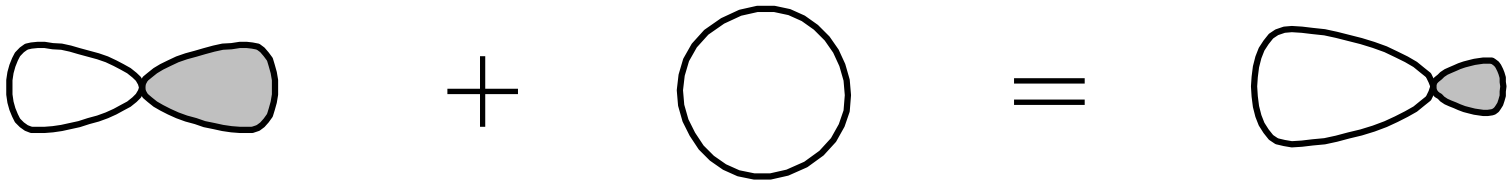


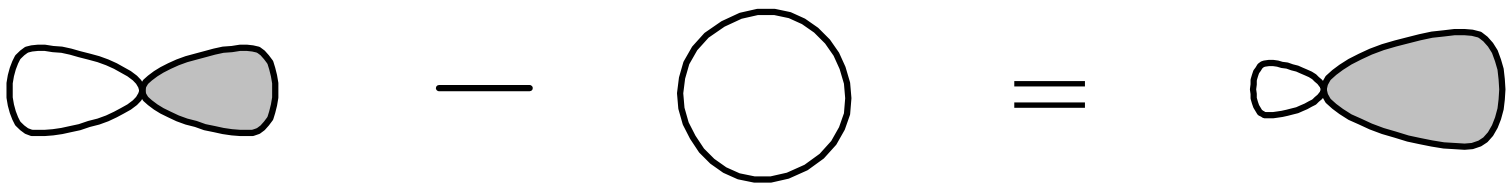
Valence-bond Theory: H_2





Pictorial VB Theory: sp Hybrids





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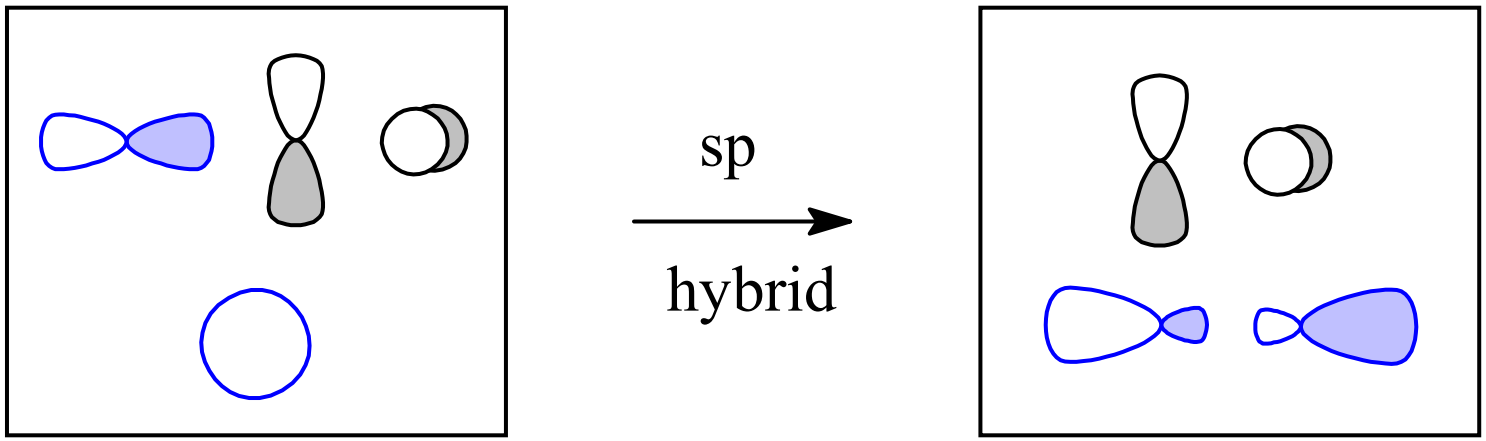
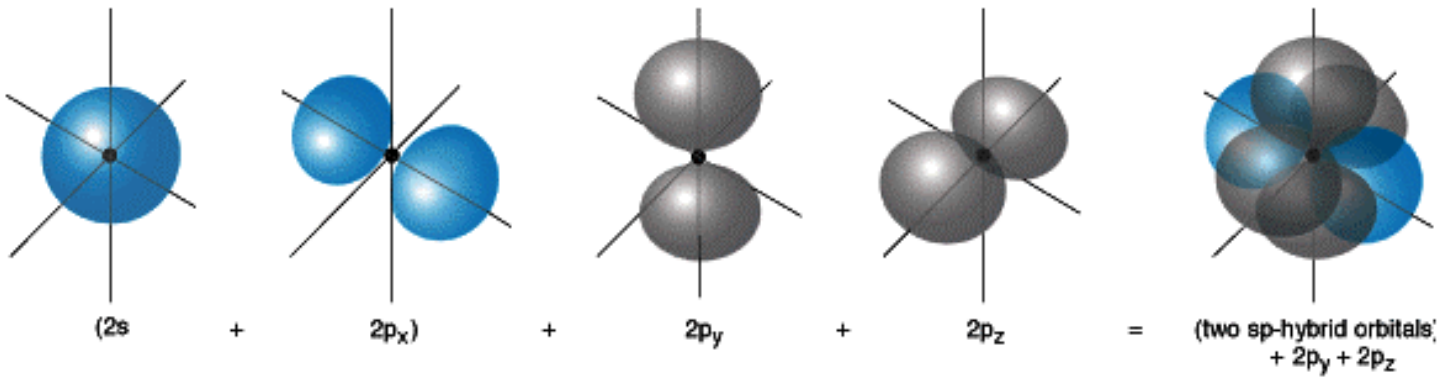
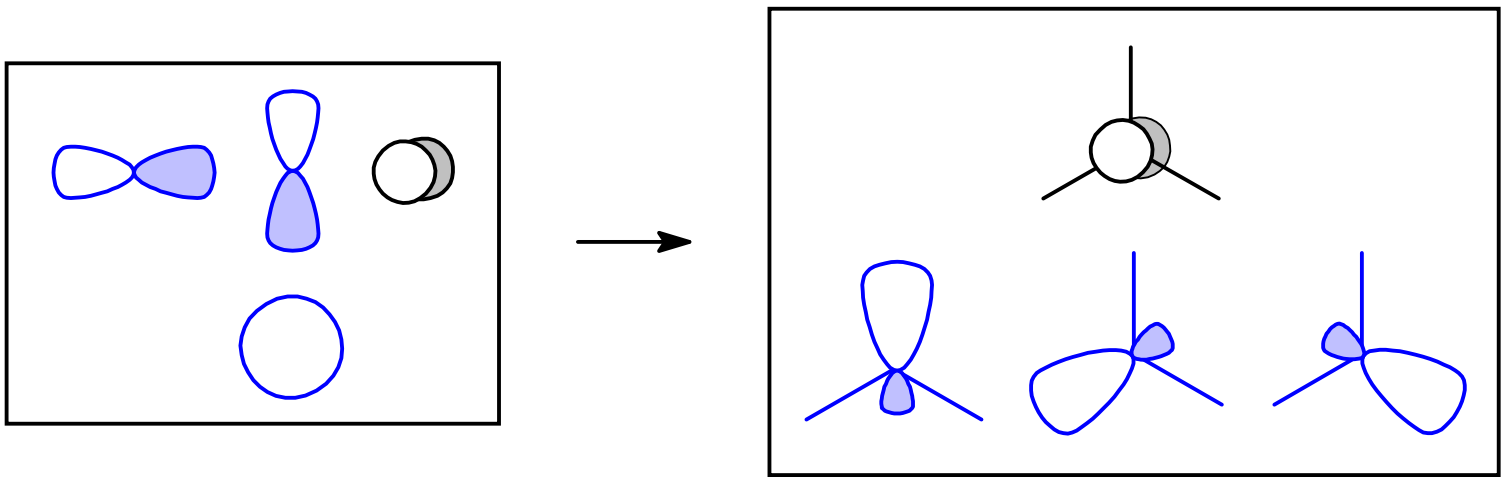
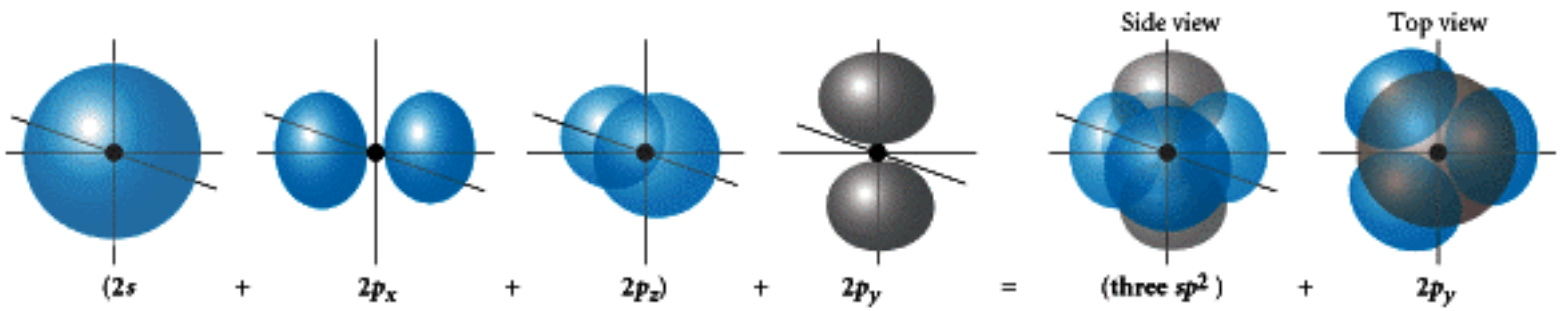


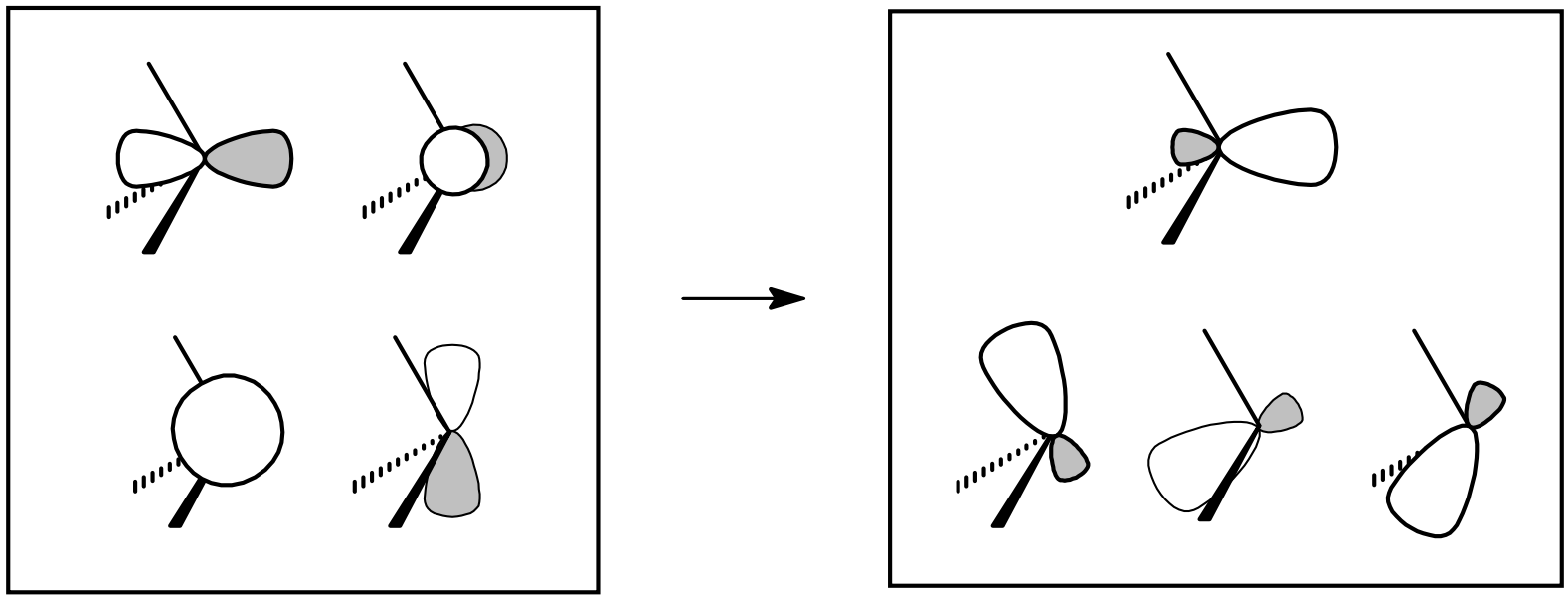


Pictorial VB Theory: sp^2 Hybrids

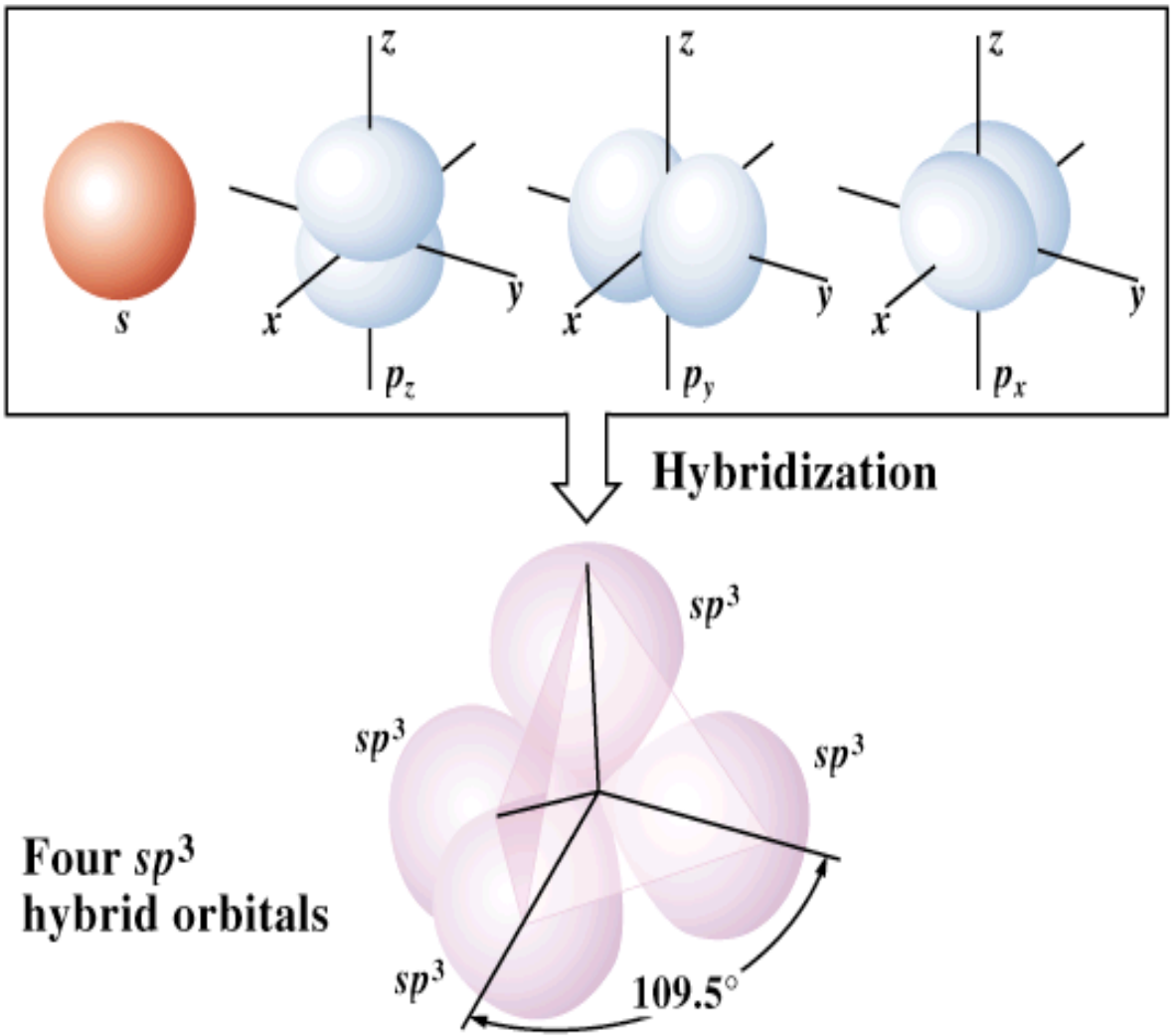




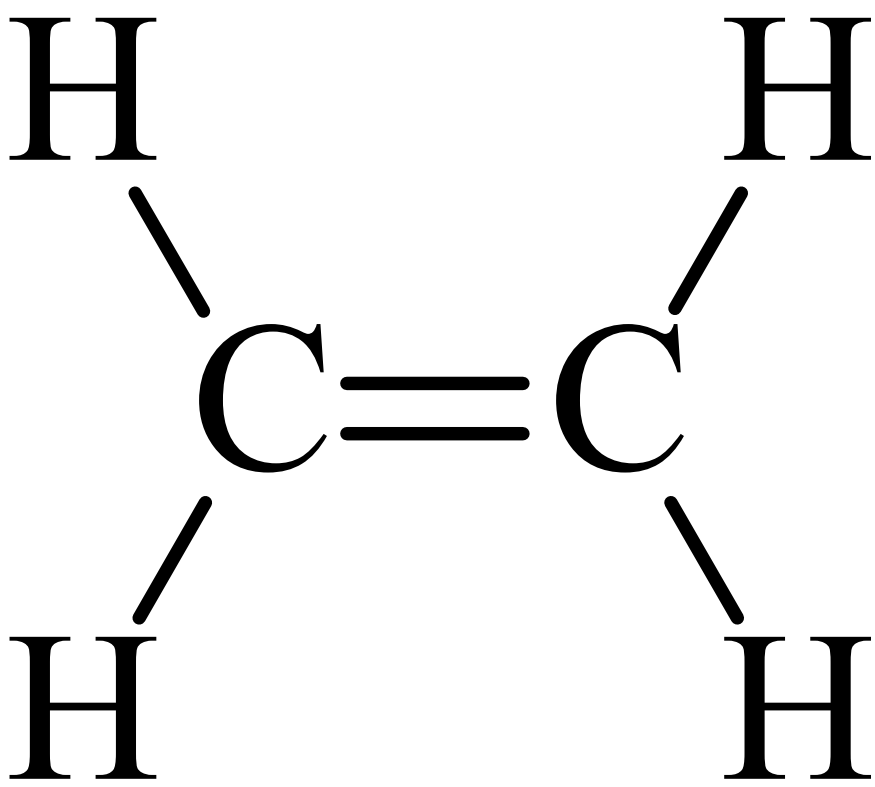
Pictorial VB Theory: sp^3 Hybrids



Pictorial VB Theory: sp^3 Hybrids



Pictorial VB Theory: Ethene



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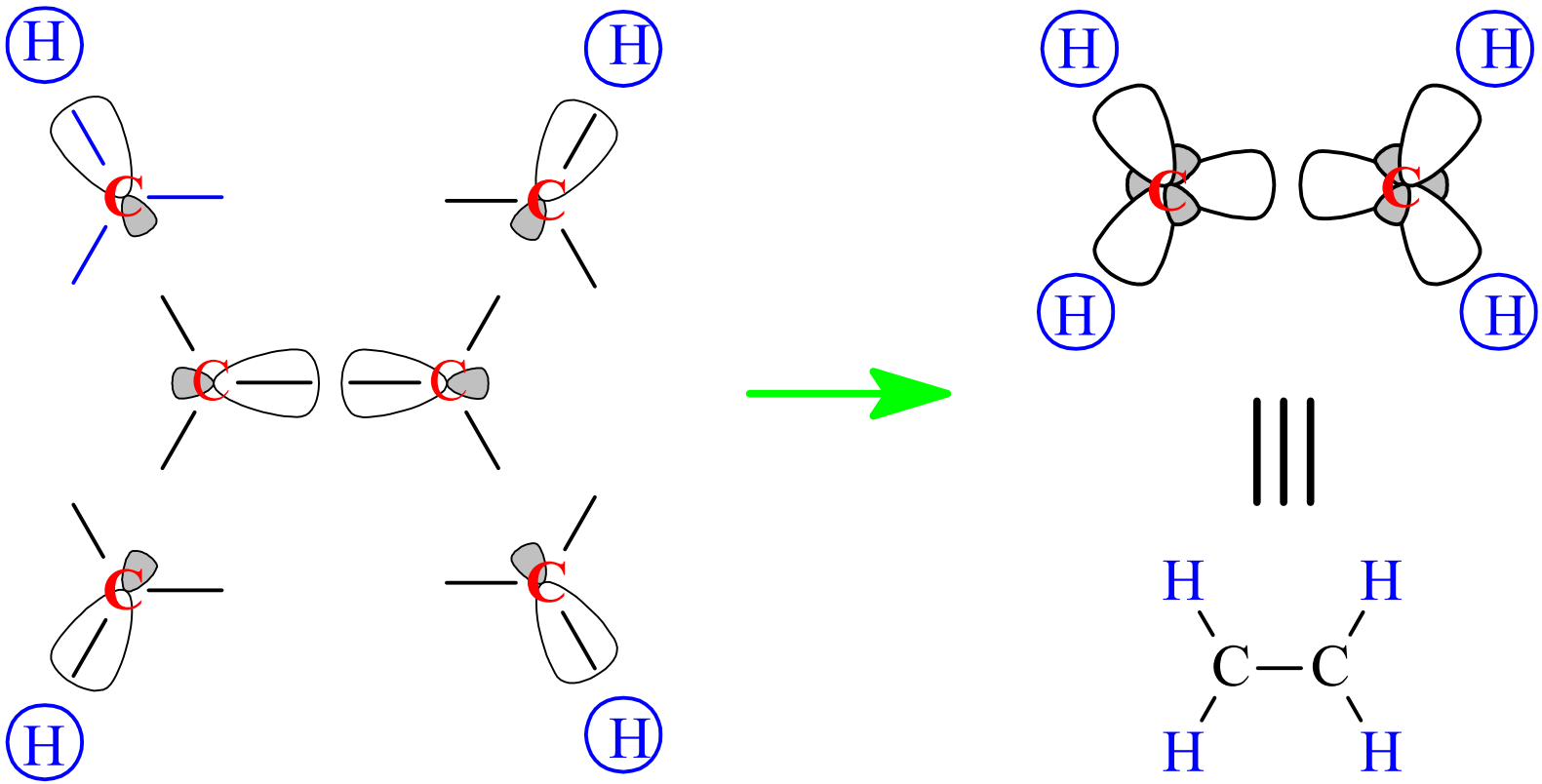

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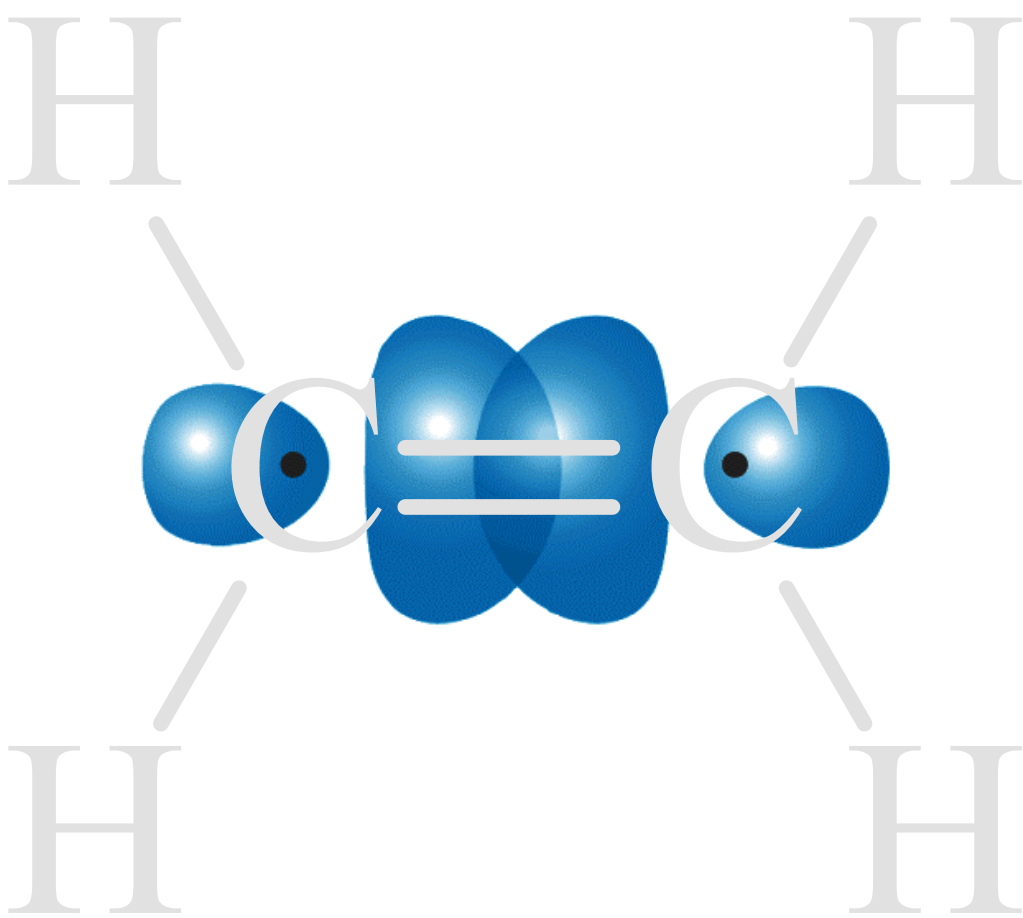
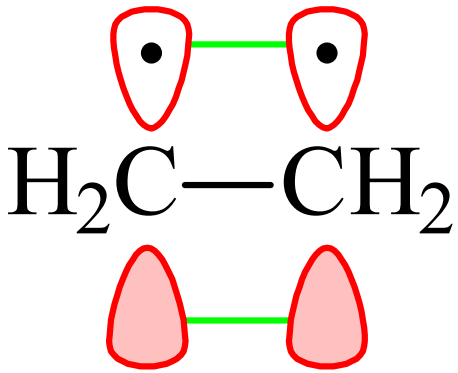


Pictorial VB Theory: Ethene



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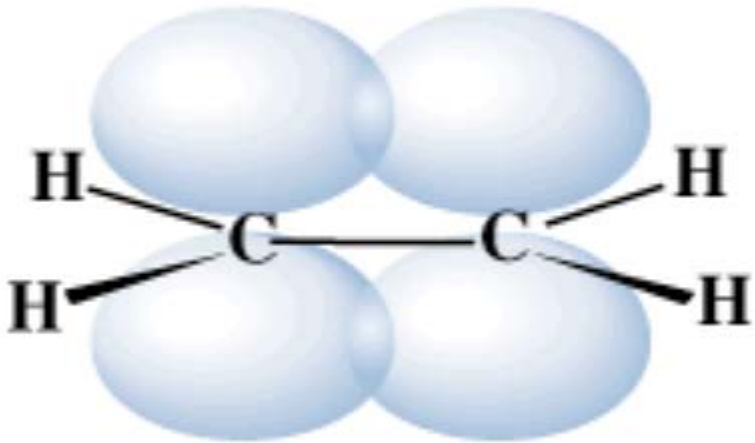
$H_2C{=}CH_2$



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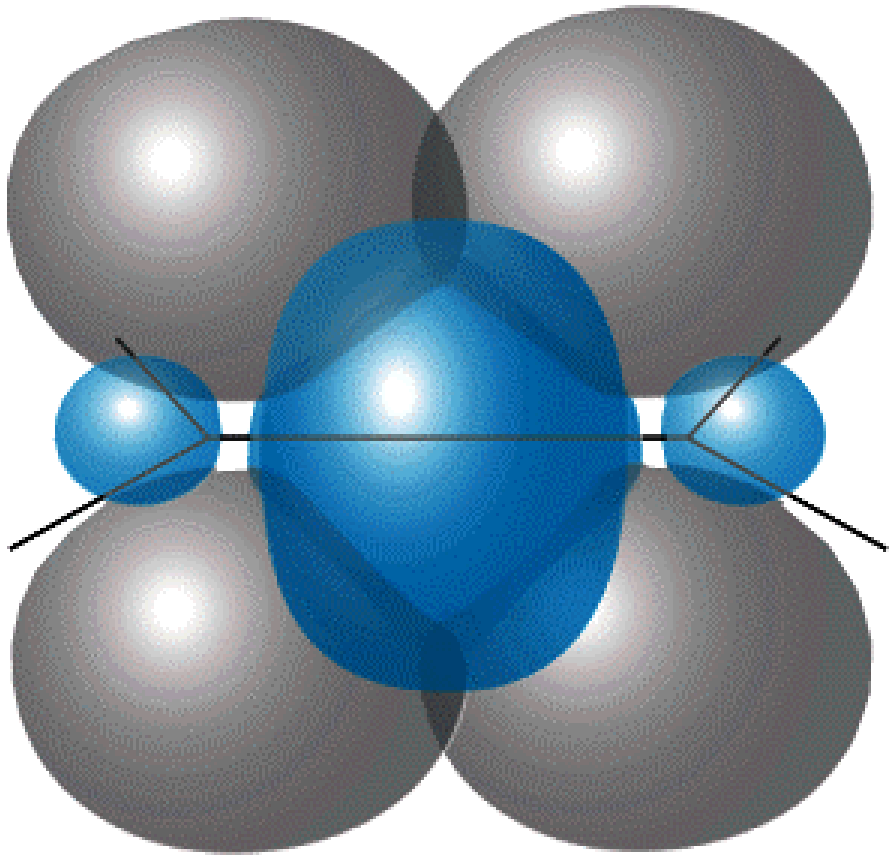
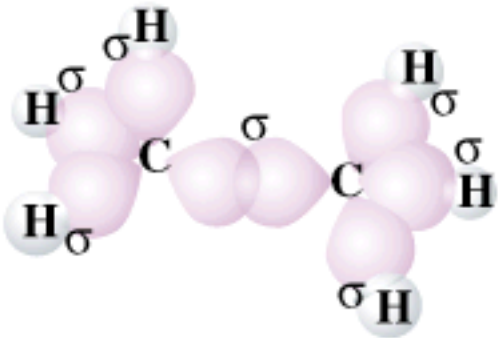
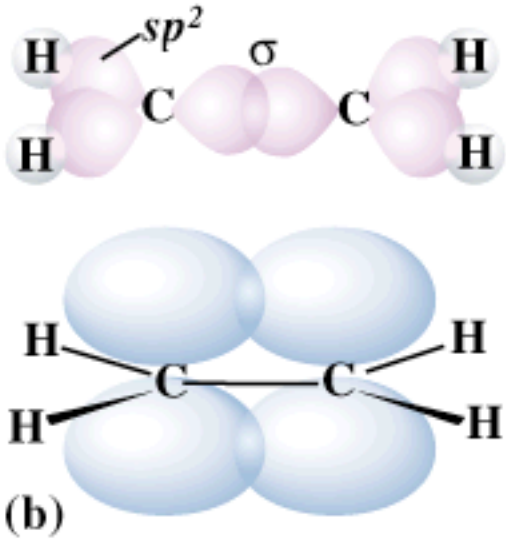


Sigma and pi bonding in ethane, ethylene, and acetylene



(a)



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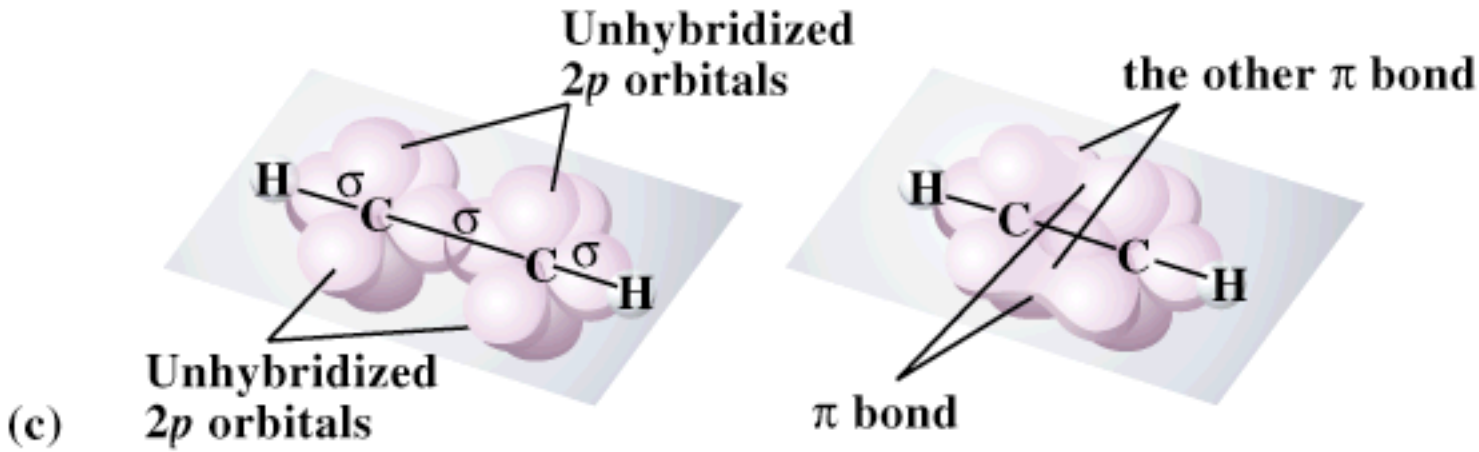
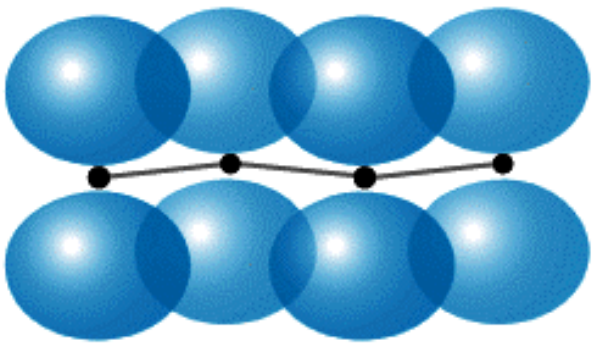


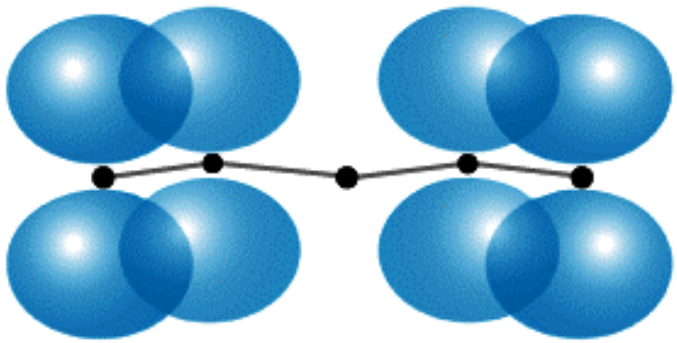
(c)

Conjugation

- Conjugated bonds: p atomic orbitals form a continuous system
- Isolated bonds: p atomic orbitals do not form a continuous system



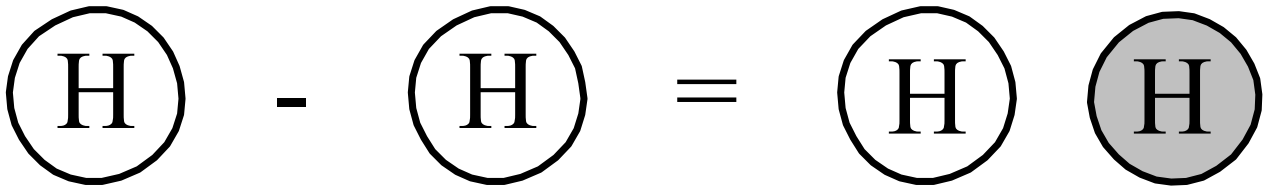
Butadiene (conjugated)

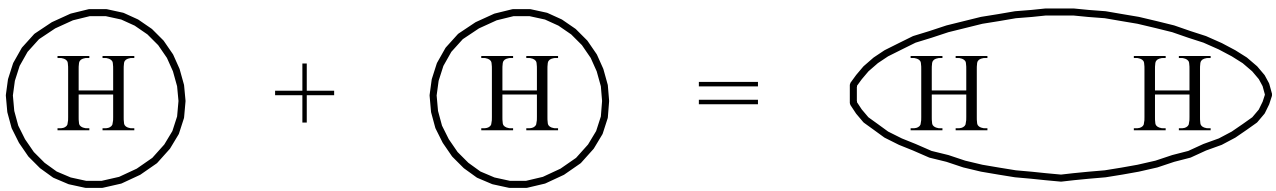


1,4-Pentadiene (isolated)

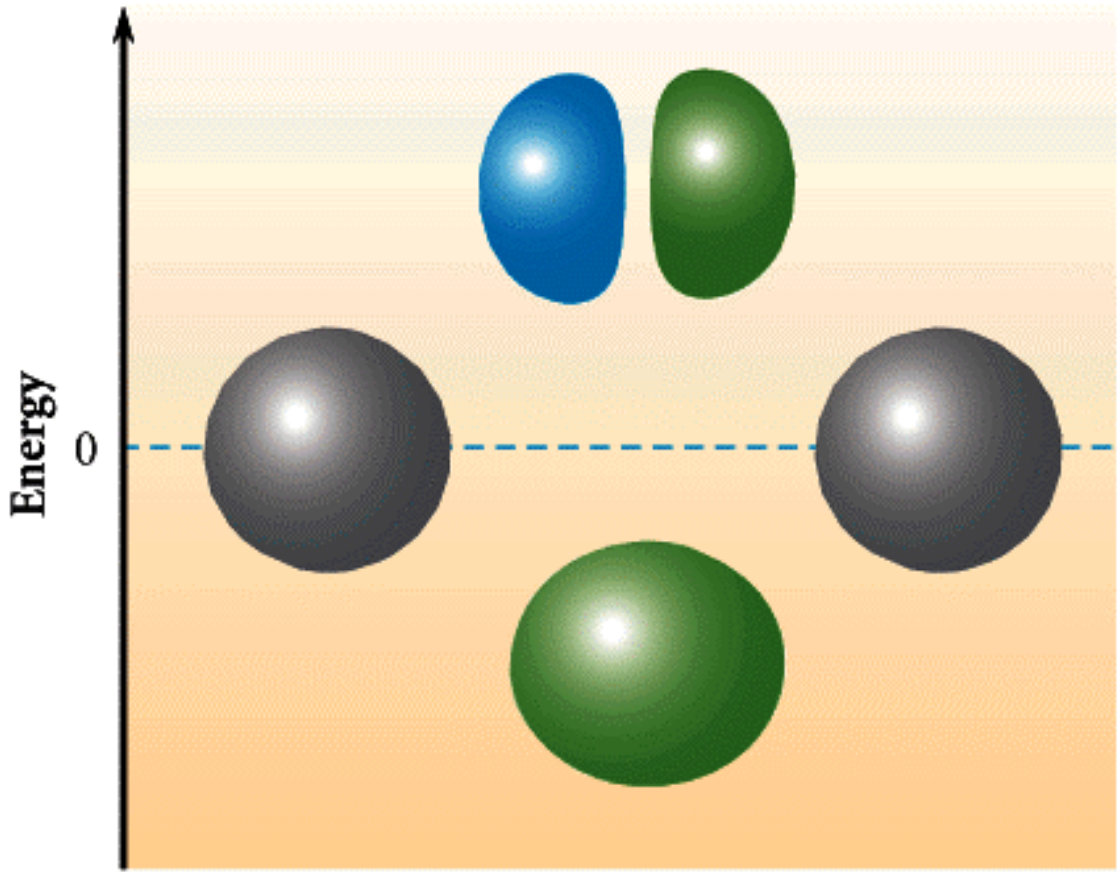
Need Molecular Orbital Theory

Molecular Orbital Theory: H_2

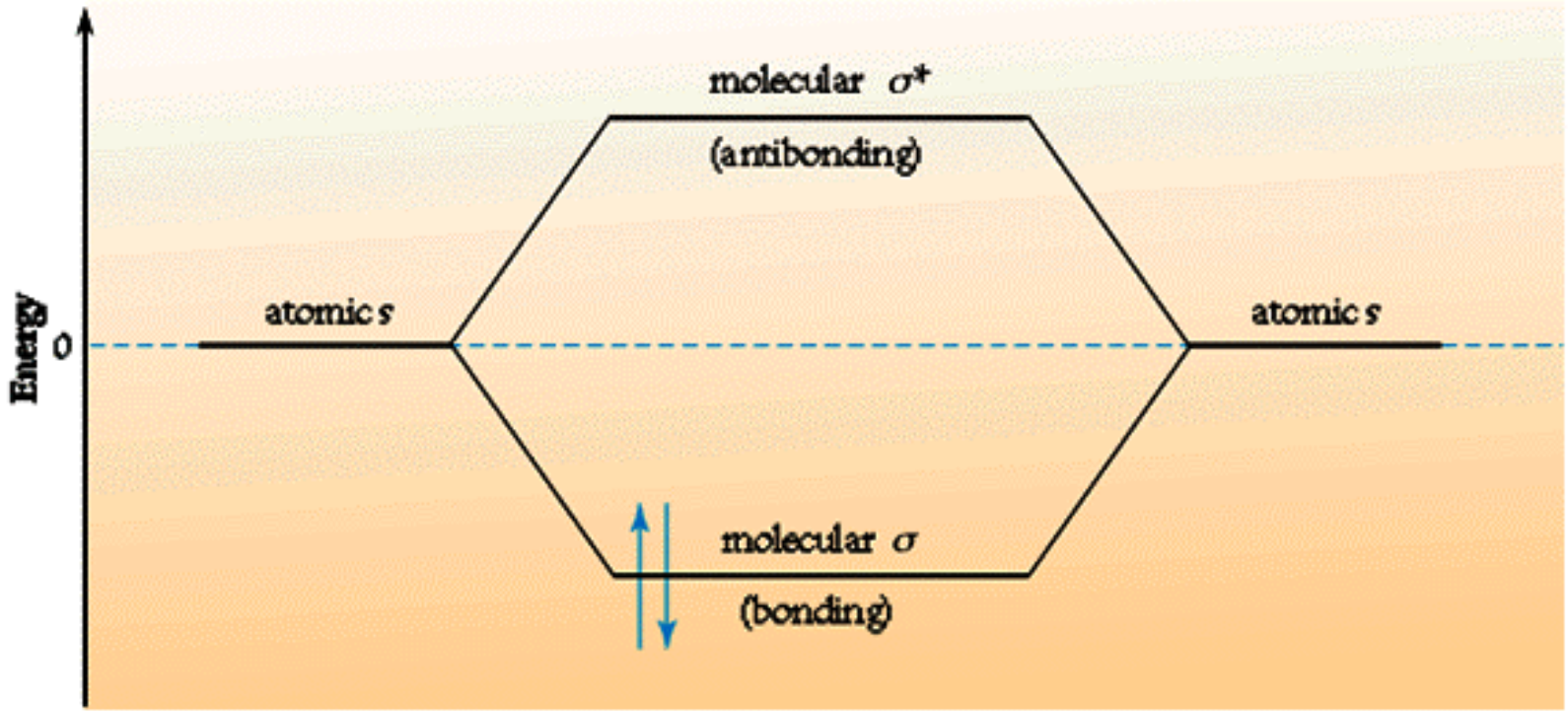




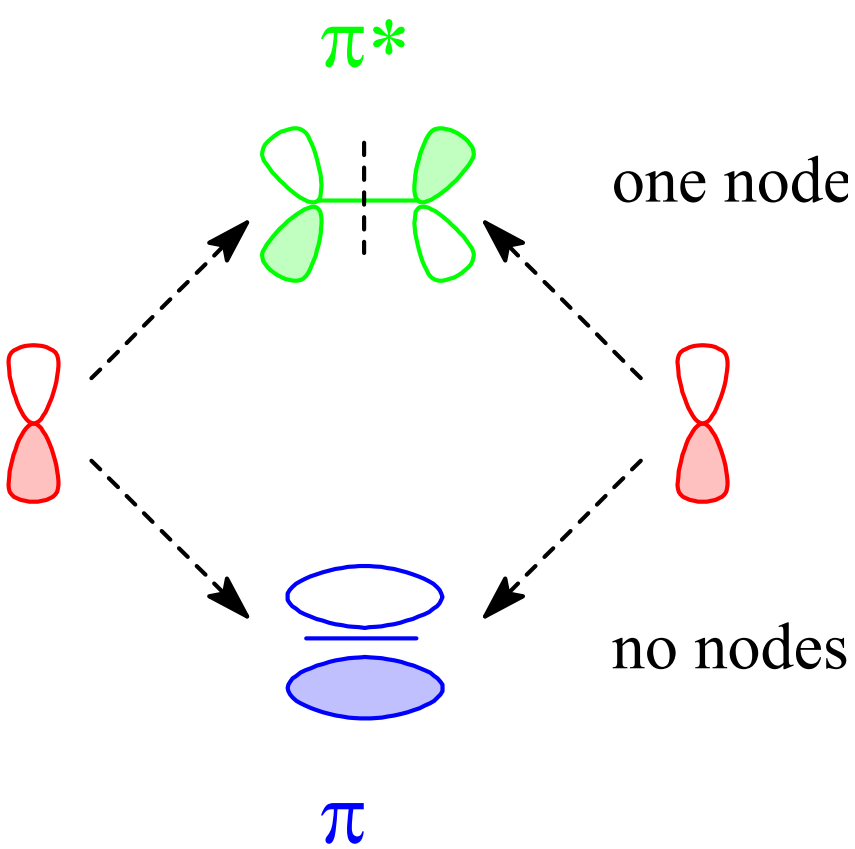
Molecular Orbital Theory: H_2

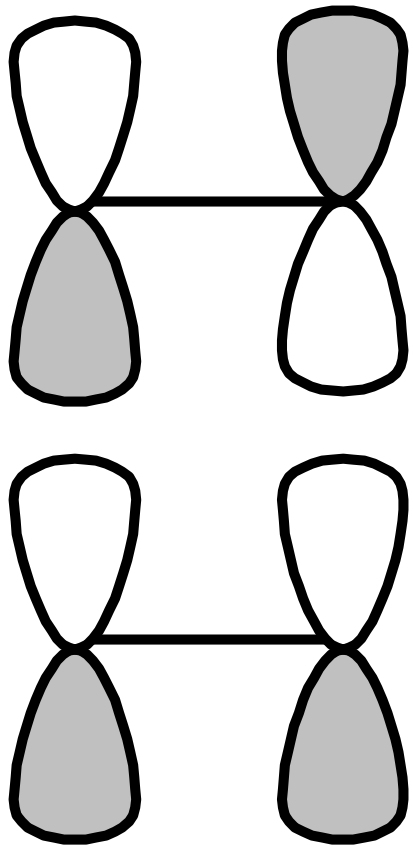


Molecular Orbital Theory: H_2



Conjugation in π-Systems: Ethene





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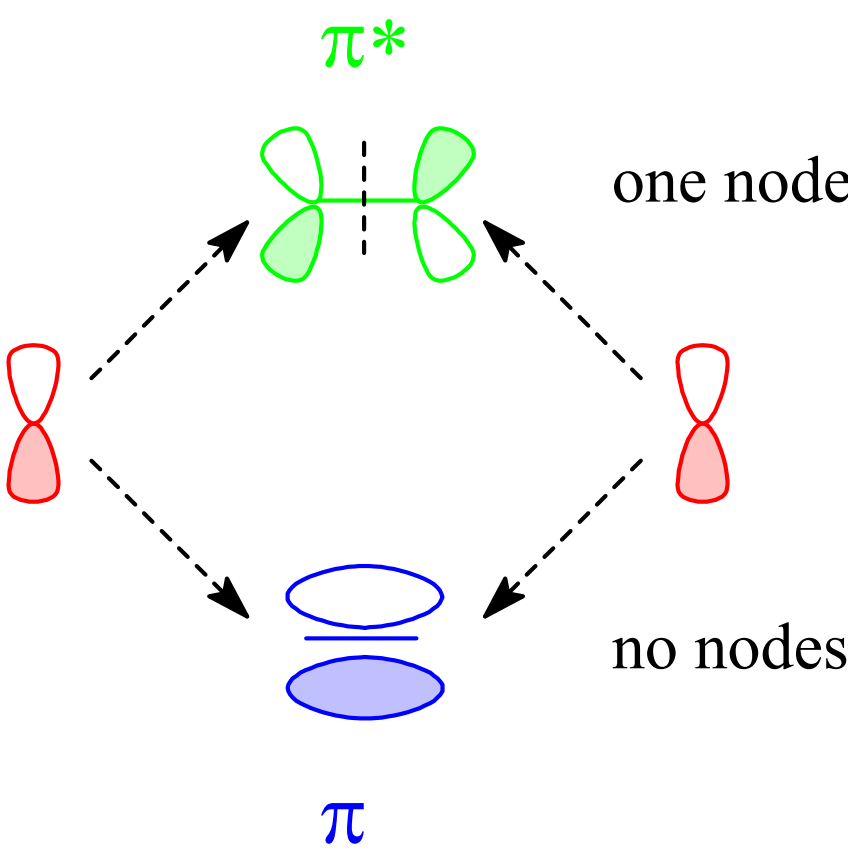
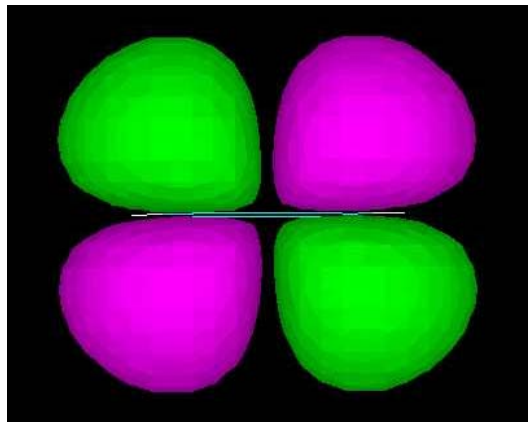
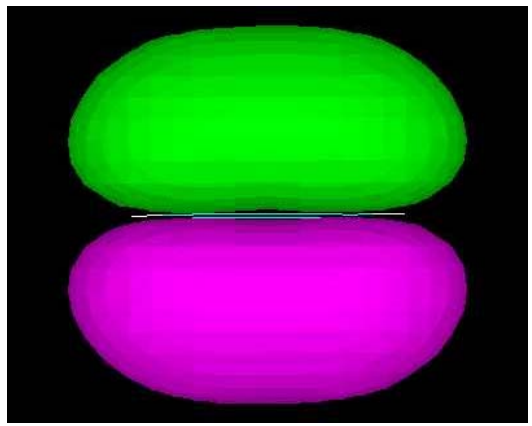
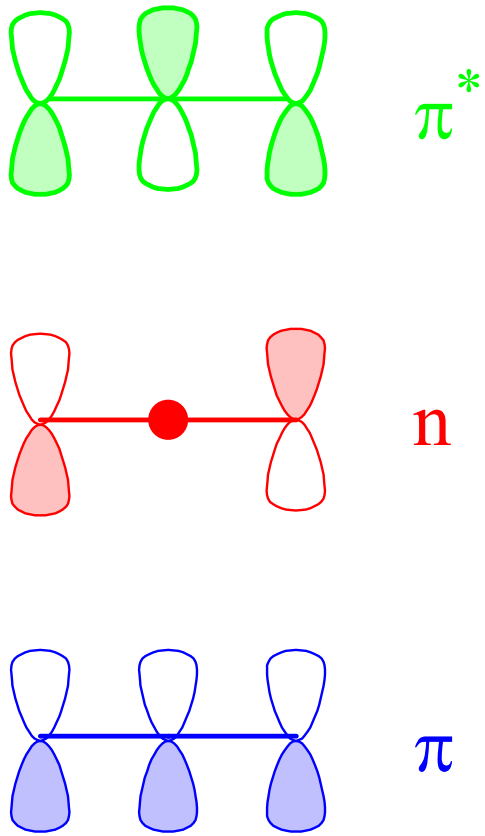
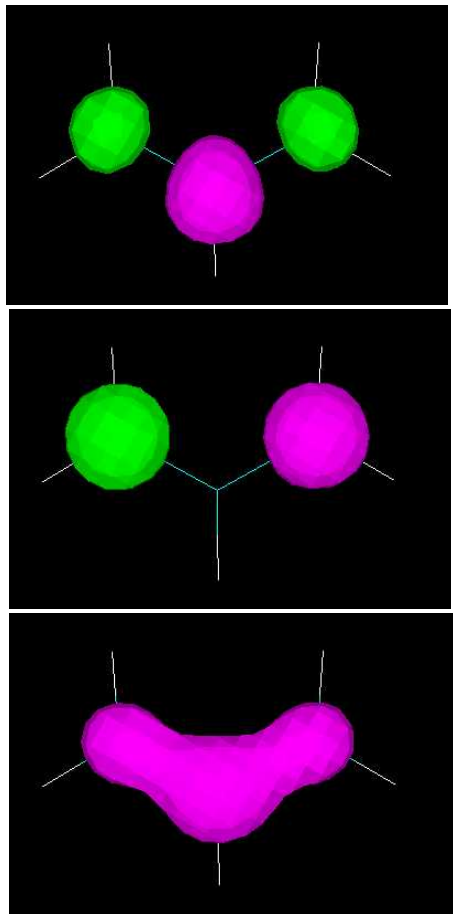




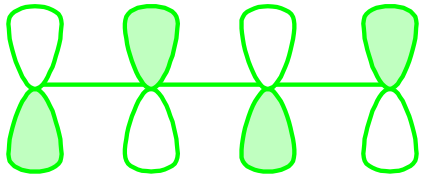


Conjugation in π-Systems: Allyl

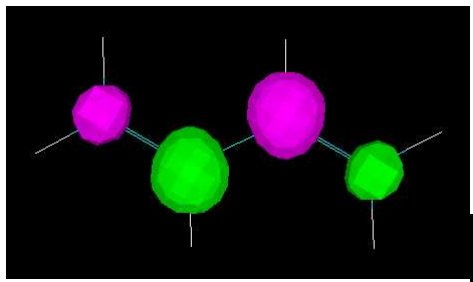


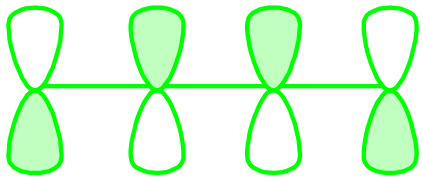


Conjugation in π-Systems: Butadiene

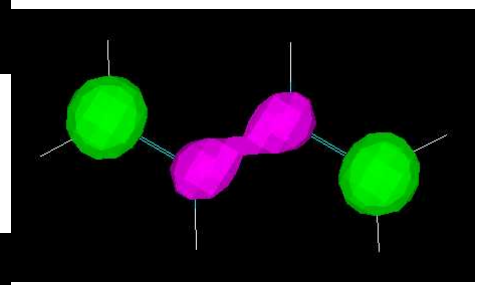


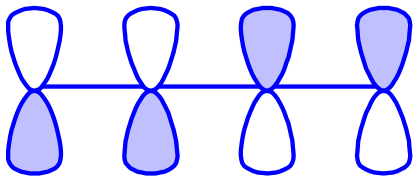
π^*



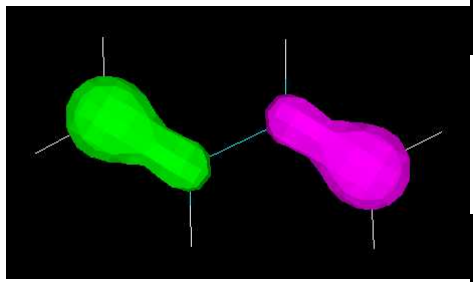


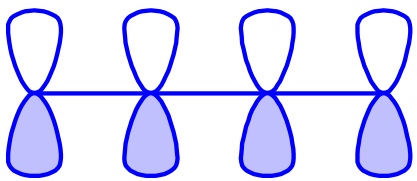
π^*



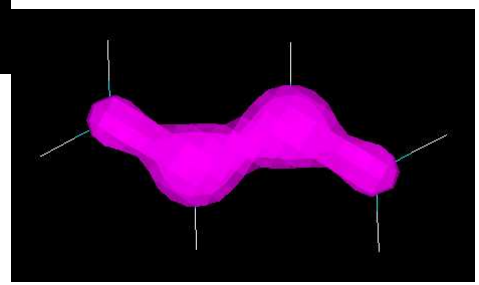


π

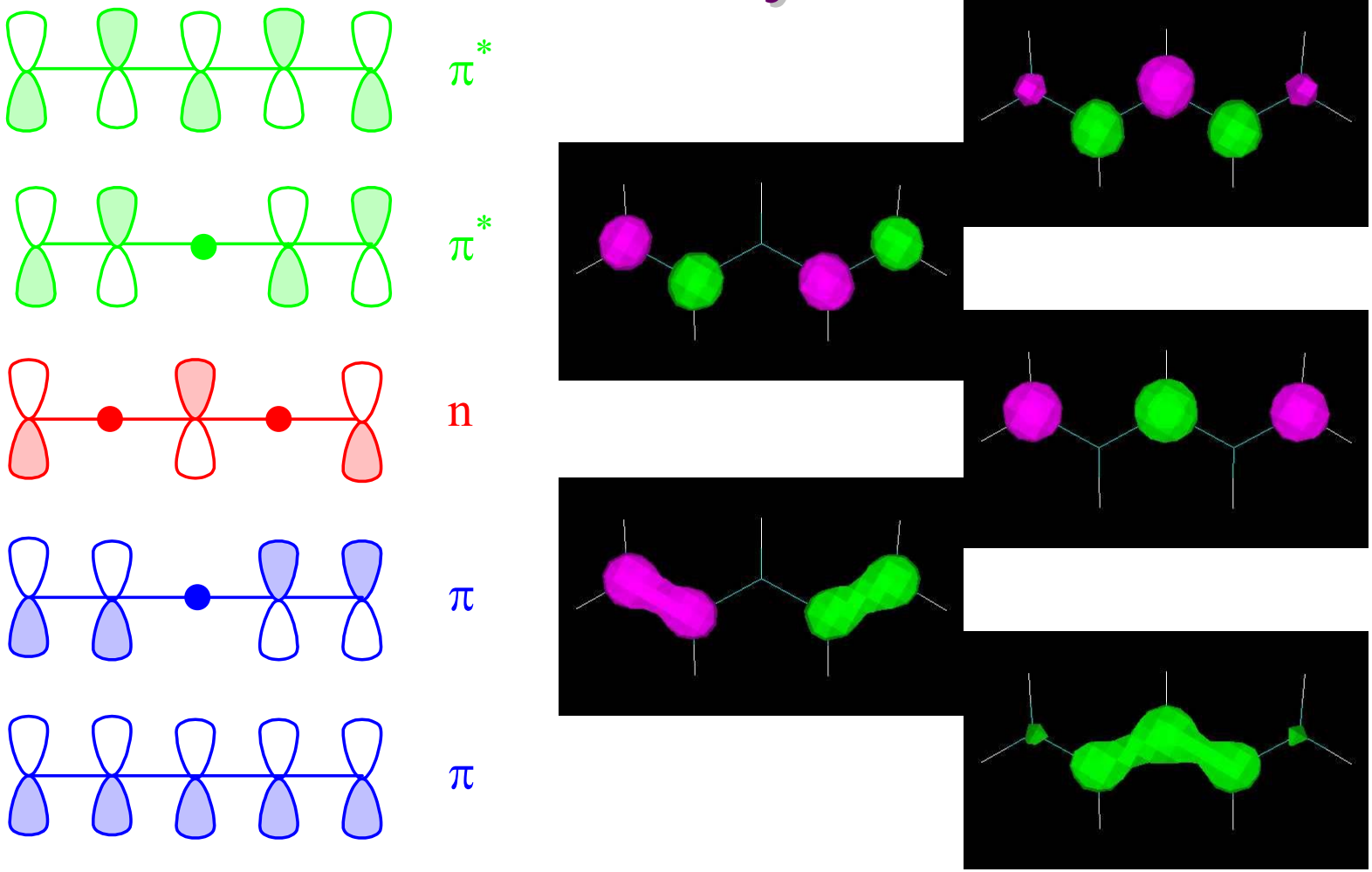




π



Conjugation in π-Systems: Pentadienyl



Conjugation in π-Systems: Hexatriene