Chapter 1:
Electronic Structure and Bonding

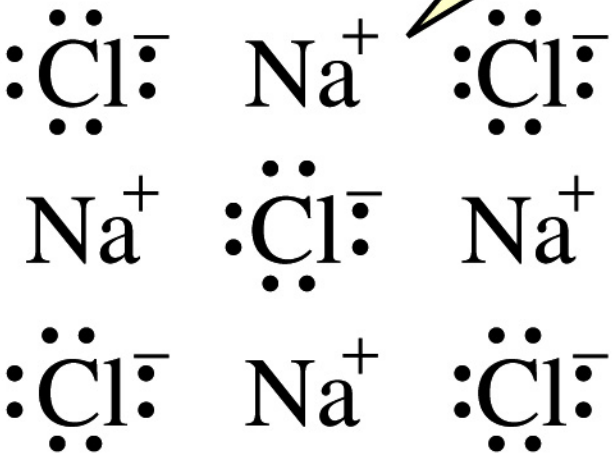
Or

A Brief Review of General Chemistry

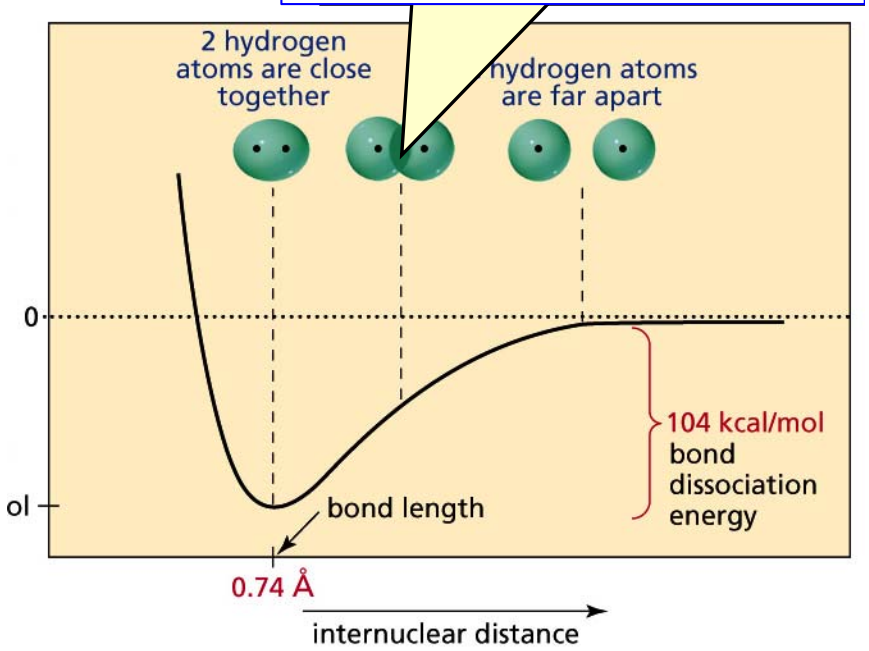
Part 2: Quantum Mechanics and Molecular Orbital Theory

Review ideas from general chemistry:
atoms, bonds, molecular geometry

Finish Chapter 1

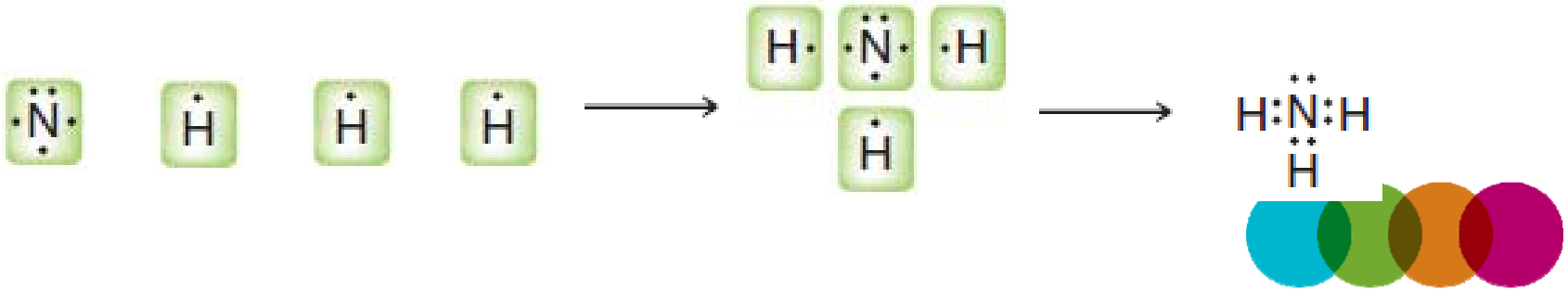


sodium chloride



Electronic Structure and Bonding

- For simple Lewis Dot structures:
- Take NH_3, for example:



Electronic Structure and Bonding

Lewis Dot Structures

- Each valence electron is indicated by a dot.
- Hydrogen wants to have 2 electrons.

- Propane – C_3H_8

Electronic Structure and Bonding

Lewis Dot Structures

- What about non-bonding electrons?
- Ethanol – C_2H_6O

Electronic Structure and Bonding

Formal charge =
number of valence electrons -
number of lone pair electrons - 1/2 number of shared electrons)

Hydronium Ion, H_3O^+

Methyl ammonium chloride (CH_3NH_3Cl)

Electronic Structure and Bonding

Rules for Lewis Dot Structures:

1. All valence electrons are shown

Total e^- = Sum of all valence electrons on all atoms involved

2. Determine connectivity. COH or OCH?
3. Add & subtract electrons for anionic and cationic charges, respectively.
4. Complete octet for each atom to fullest extent possible.

Electronic Structure and Bonding

Bonding Models

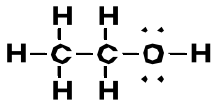
- Lewis structures – Uses dots to show covalent bonds & non-bonding valence electrons (CH_3COOH)

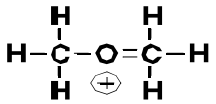
- Kekulé line structures – Use of lines to show covalent bond(s)

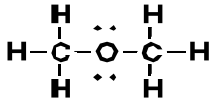
- Condensed structures – eliminates all lines & dots

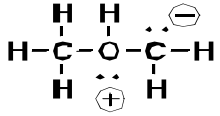
- Organic structures – use of corners to show carbons, fill in other elements

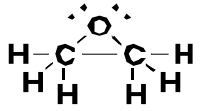
Which of the following is(are) not possible Lewis Structure(s) for C_2H_6O?

a. 

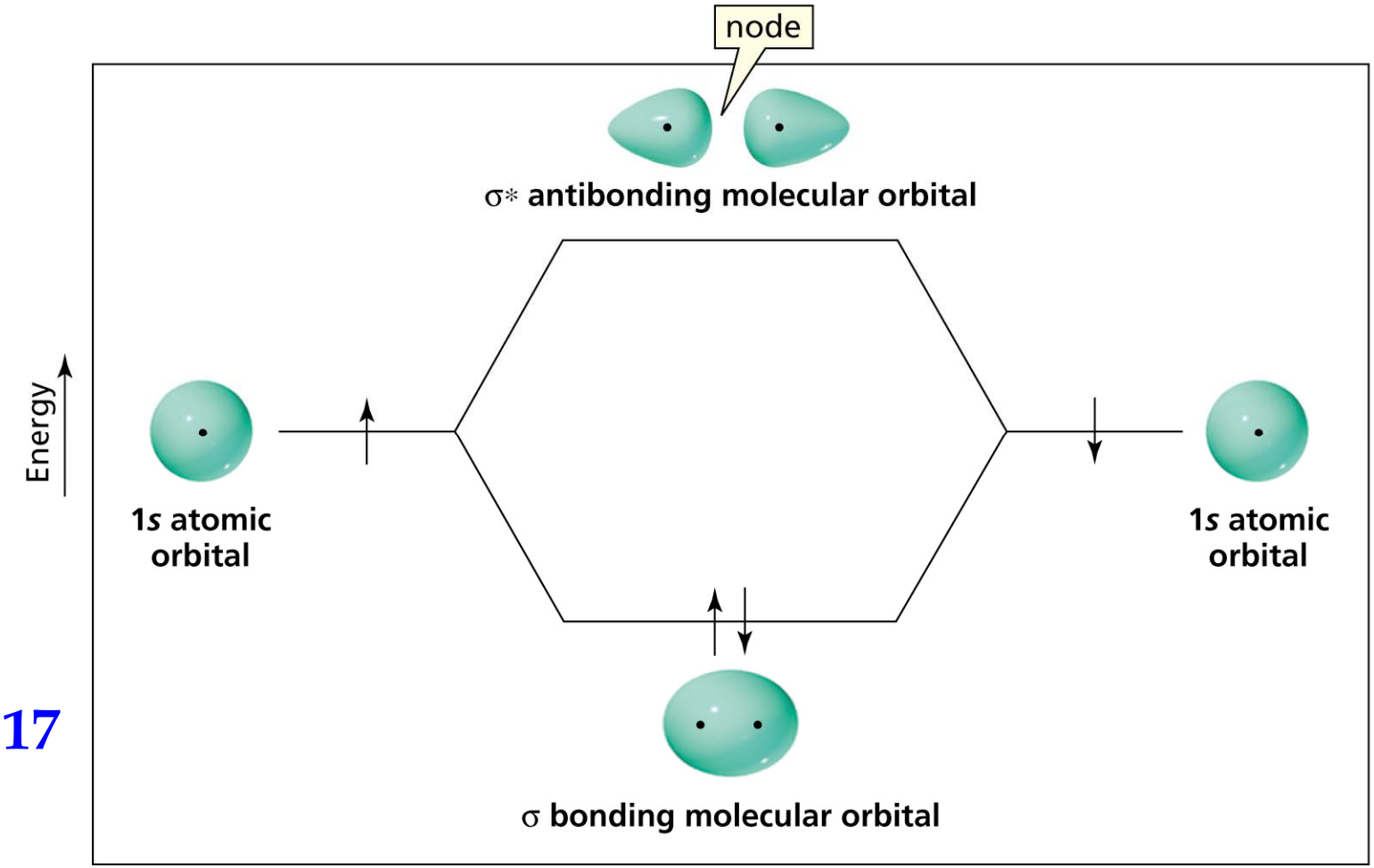
b. 

c. 

d. 

e. 

Molecular Orbital Theory



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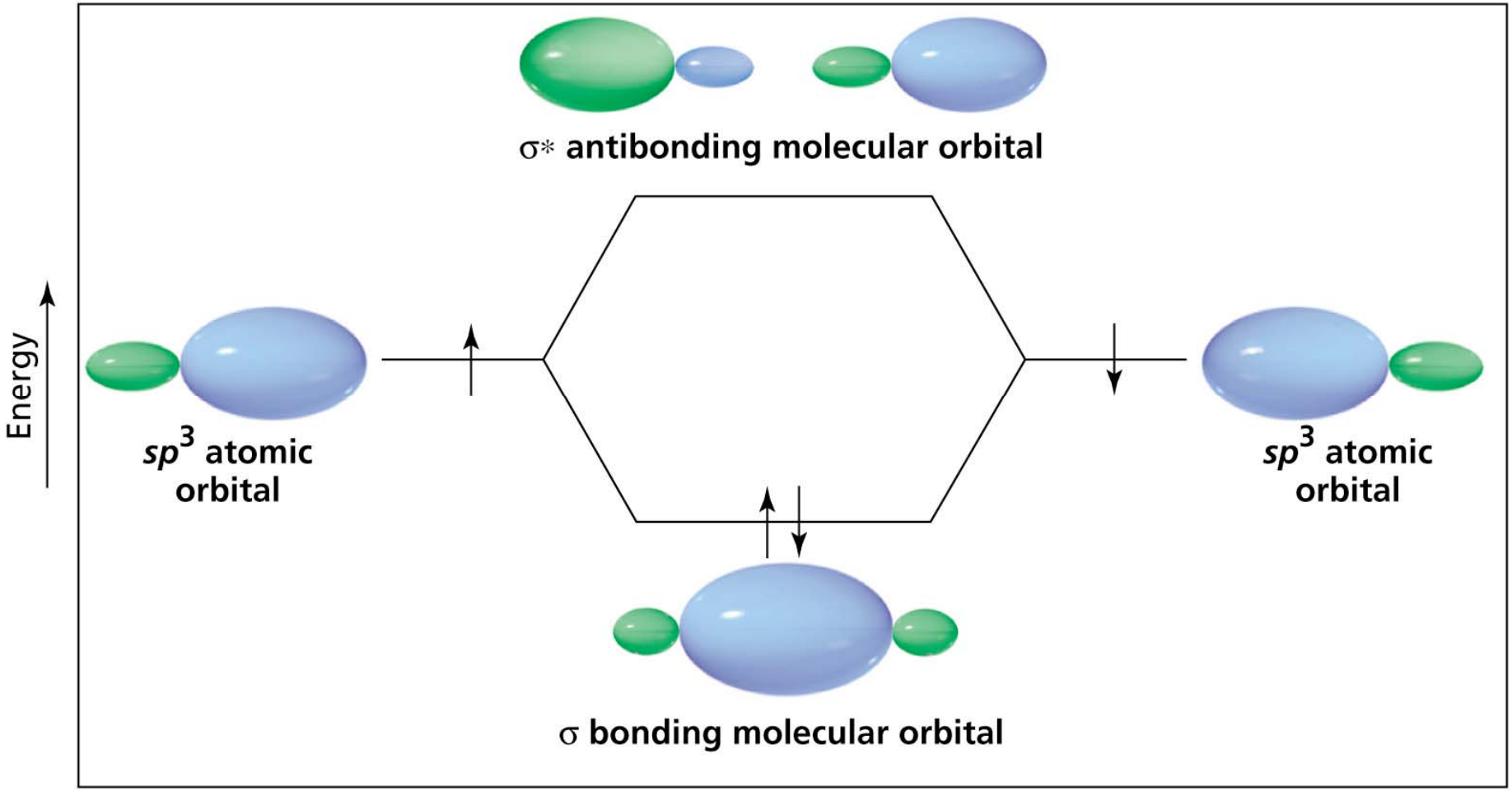
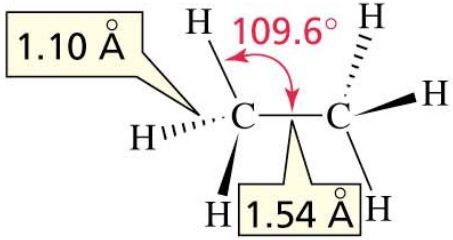
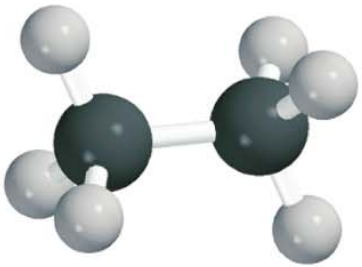
Hybrid Orbitals of Ethane, C_2H_6

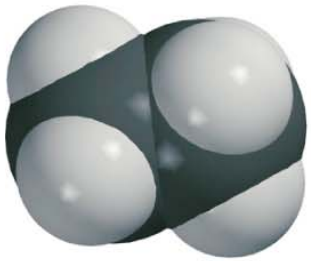


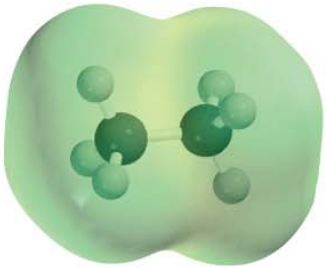
Hybrid Orbitals of Ethane, C_2H_6



perspective formula of ethane


ball-and-stick model of ethane


space-filling model of ethane


electrostatic potential map for ethane

- _____ which overlap to form the C-C bond are shaped such that rotation about the bond axis does not interfere with their overlap.
- Structures that differ only in rotation about a single bond are called

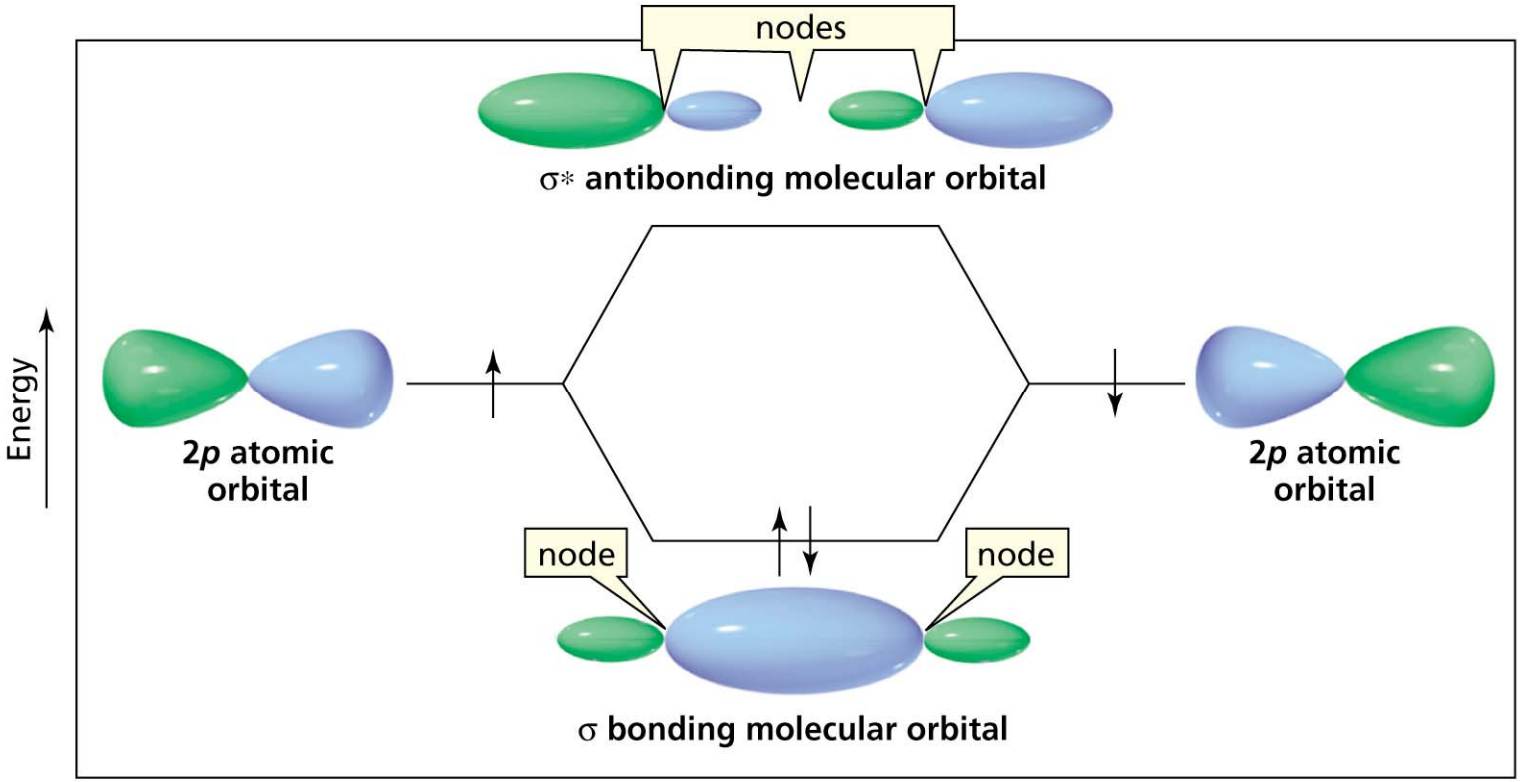
Molecular Orbital Theory

So let's look at Ethene (Ethylene) . . .

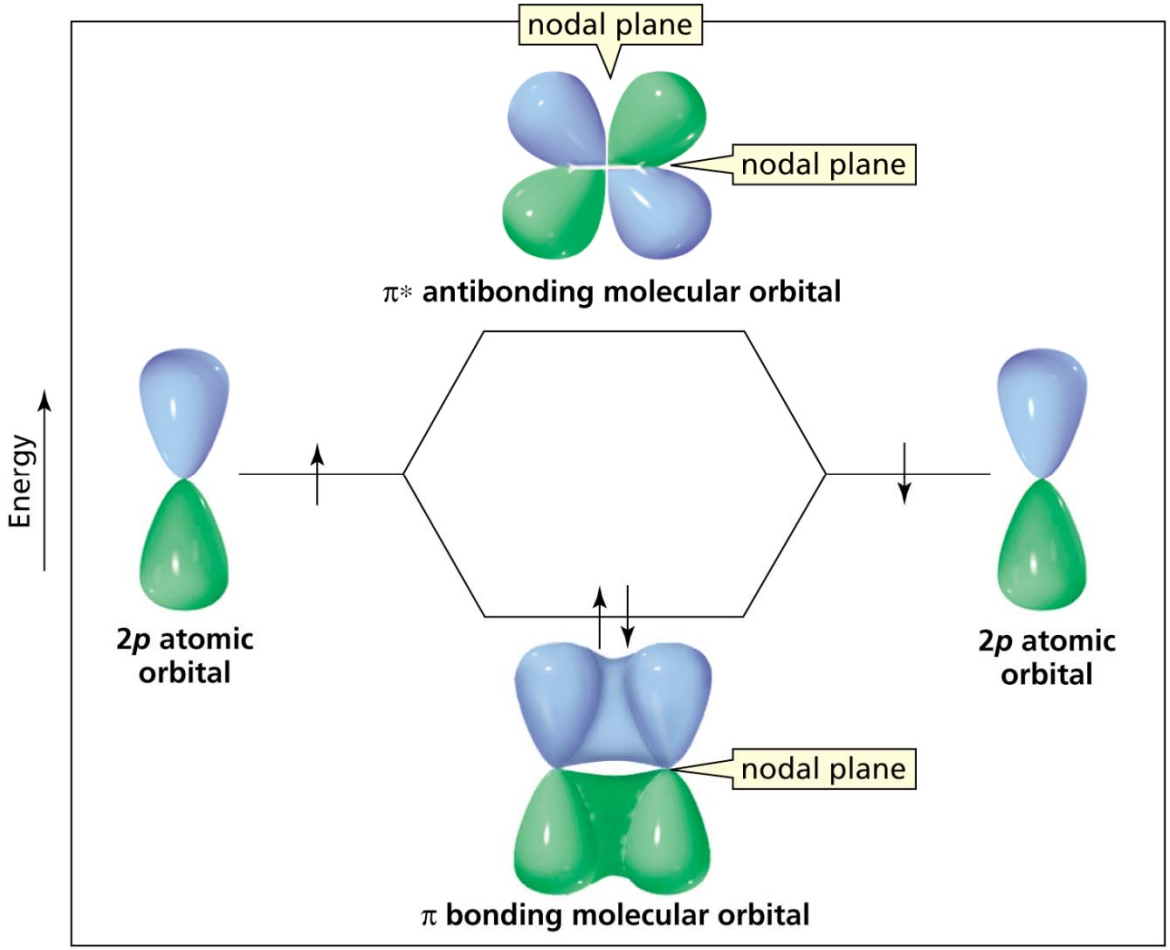
CH_2CH_2

Draw a Lewis Dot Structure for Ethene

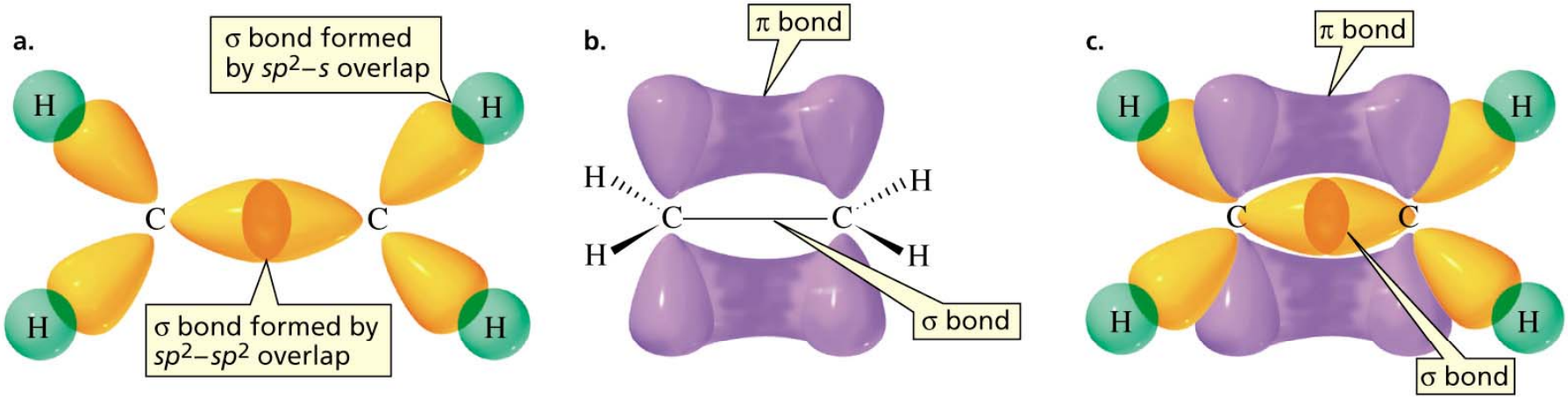
Hybrid Orbitals of Ethene, C_2H_4



Hybrid Orbitals of Ethene, C_2H_4



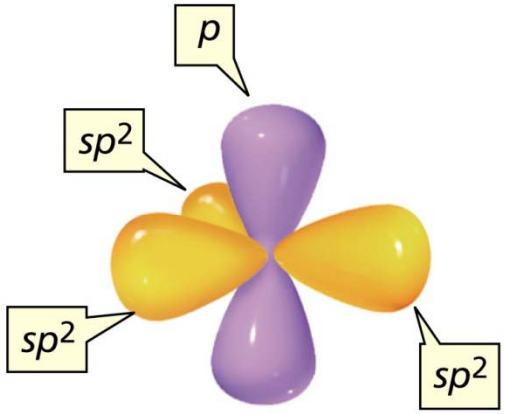
Hybrid Orbitals of Ethene, C_2H_4



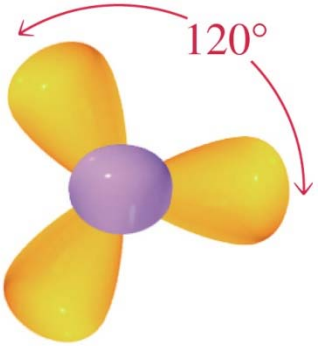
Bonding in Ethene (Ethylene): A Double Bond

- The sigma bond is unaffected by rotation of one of the CH_2 groups.

Hybrid Orbitals of Ethene, C_2H_4



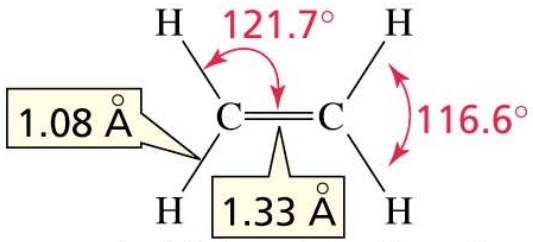
side view



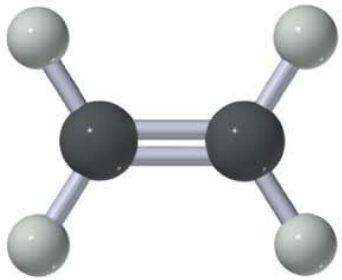
top view

An *sp*²-Hybridized Carbon -

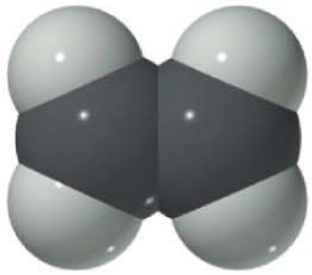
- The bond angle in the *sp*² carbon is 120˚.
- The *sp*² carbon is the trigonal planar carbon



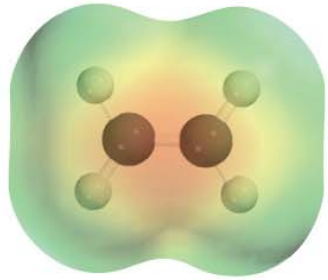
a double bond consists of one σ bond and one π bond



ball-and-stick model of ethene



space-filling model of ethene



electrostatic potential map for ethene

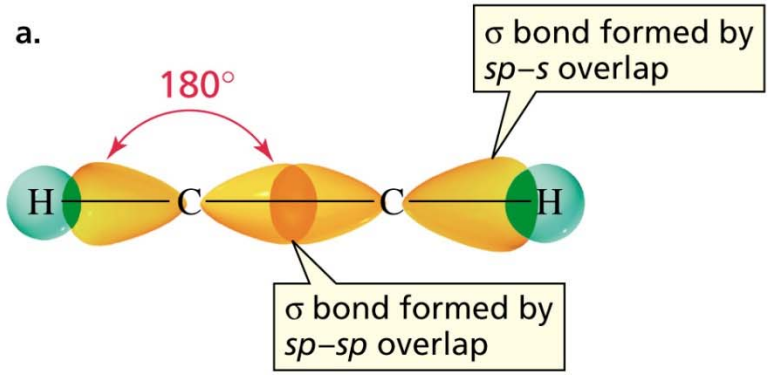
Molecular Orbital Theory

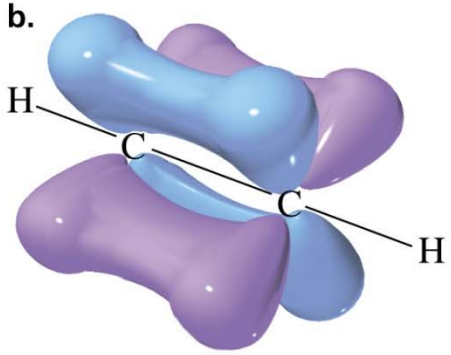
So let's look at Ethyne (Acetylene) . . .

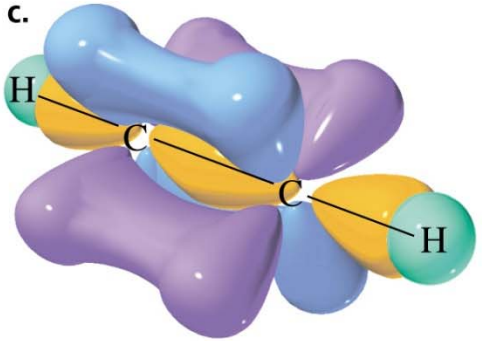
CHCH

Draw a Lewis Dot Structure for Ethyne

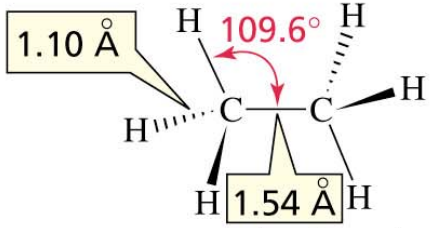
Hybrid Orbitals of Ethyne, C_2H_2



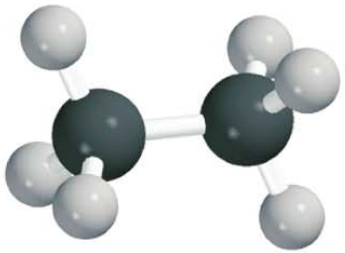




Molecular Orbital Theory



perspective formula of ethane



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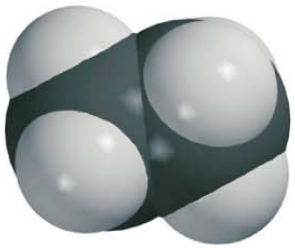
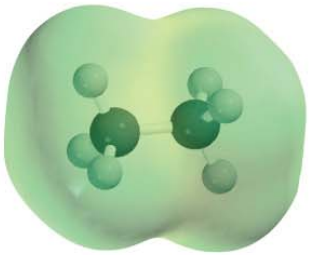
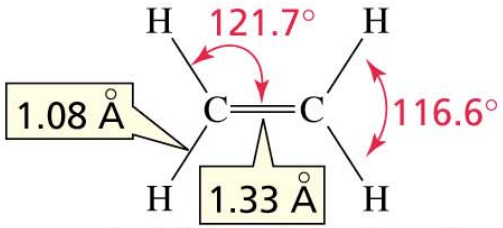


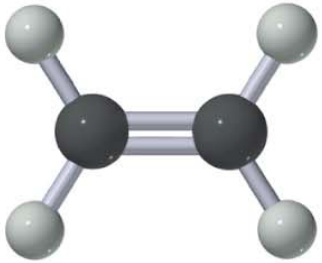
space-filling model of ethane



electrostatic potential map for ethane

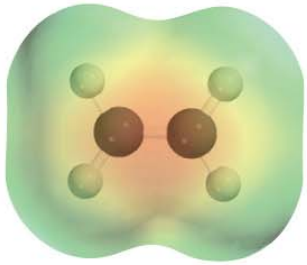


a double bond consists of one σ bond and one π bond



ball-and-stick model of ethene

space-filling model of ethene



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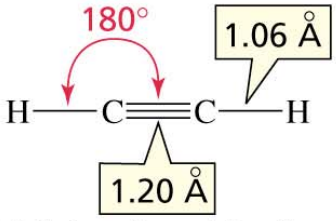
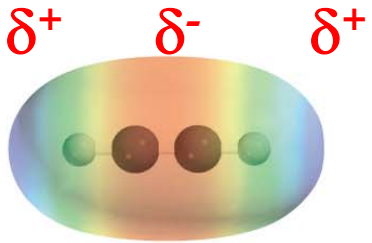


a triple bond consists of one σ bond and two π bonds

ball-and-stick model of ethyne

space-filling model of ethyne



electrostatic potential map for ethyne

Molecular Orbital Theory

Summary

For Next Time….

- Wednesday Chapter 2 Sections 2.1-2.7

- Homework Practice Problems Chapter 1

  #8,12,15,37,39,43,45,48,49,53,56

- Homework Practice Problems Chapter 2

  #1,5,12,16,25,34,40,47,48,54,55,64, 66

  *know the functional groups in table 2.1