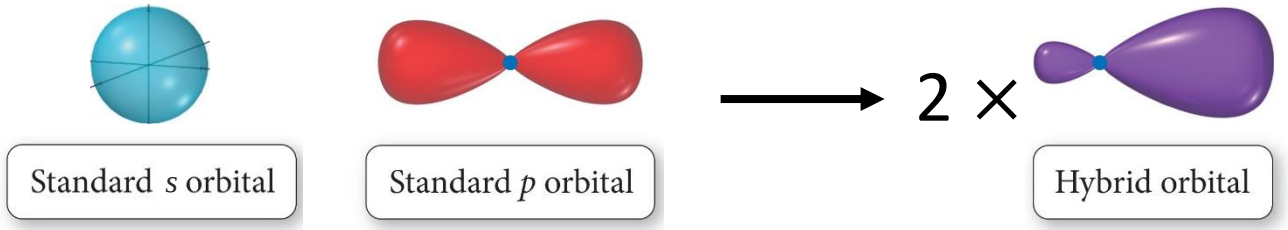
Announcements for Monday, 21OCT2024

- Week 7 Homework Assignments available on eLearning
  - Graded and Timed Quiz 7 – “Bonding” due **tonight at 6:00 PM (EDT)**
- **Exam 2 Conflict Exam Requests due by Friday, 25OCT2024, 11:59 PM (EDT)**
  - for students having Rutgers sanctioned classes and activities during the Exam 2 period (Wednesday, 30OCT2024, 7:45 PM – 9:05 PM)

ANY GENERAL QUESTIONS? Feel free to see me after class!

Hybridization Theory

- usually focuses on the valence orbitals of central/interior atoms in molecules
- an atom "mixes" some of its "regular" valence orbitals to form new **hybrid** orbitals
  - atomic orbitals can be mixed in different proportions
- the shapes and energies of the hybrid orbitals are between the shapes and energies of the unhybridized orbitals



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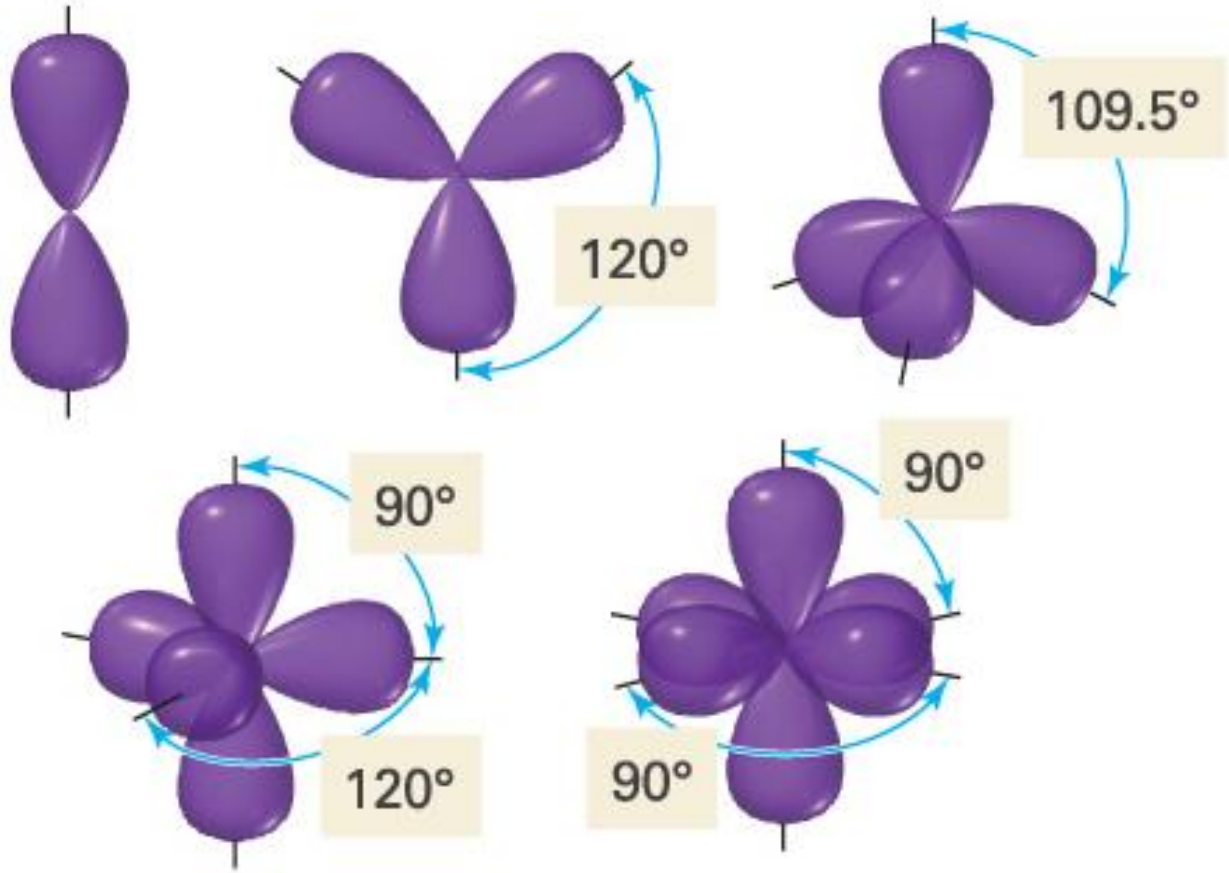
- the number of identical hybrid orbitals formed equals the number of unhybridized orbitals mixed to make the hybrids
  - example: 4 atomic orbitals go in, 4 hybrid orbitals are produced
- the arrangement of hybrid orbitals around the central atom gives the same electron group geometries and shapes predicted by VSEPR
- hybrid orbitals can be used to make **sigma bonds (?!?)** and to hold lone pairs or single electrons

Hybridization and Electron Groups

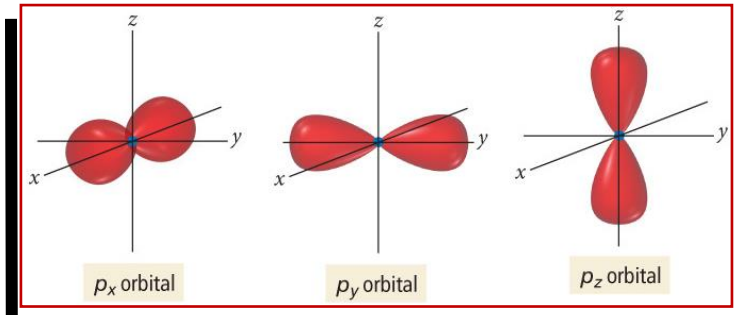
the number of electron groups around the central atom tells you the atom's hybridization

- 2 e^- groups = sp hybridization
  - **linear** arrangement of hybrid orbitals around the atom
- 3 e^- groups = sp^2 hybridization
  - **trigonal planar** arrangement of hybrid orbitals around the atom
- 4 e^- groups = sp^3 hybridization
  - **tetrahedral** arrangement of hybrid orbitals around the atom
- 5 e^- groups = sp^3d hybridization
  - **trigonal bipyramidal** arrangement of hybrid orbitals around the atom
- 6 e^- groups = sp^3d^2 hybridization
  - **octahedral** arrangement of hybrid orbitals around the atom



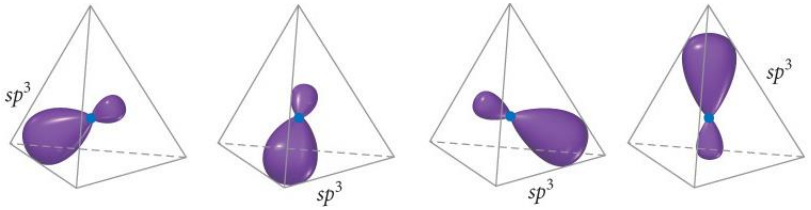
Note: For clarity, only one lobe of each hybrid orbital is being shown above

Orbital Energies: Unhybridized vs. sp^3 Hybridized

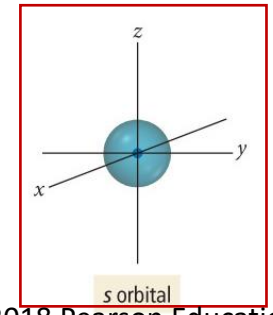


Energy ↑

hybridization →

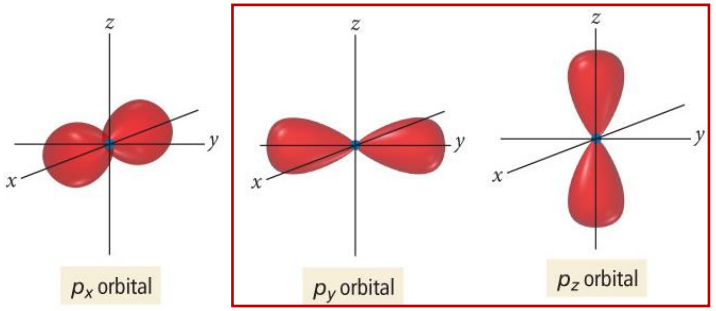


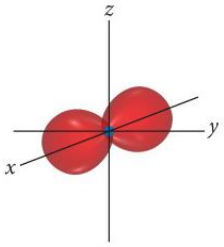
four new identical sp^3-orbitals



unhybridized **sp^3 hybridized**

Orbital Energies: Unhybridized vs. sp^2 Hybridized

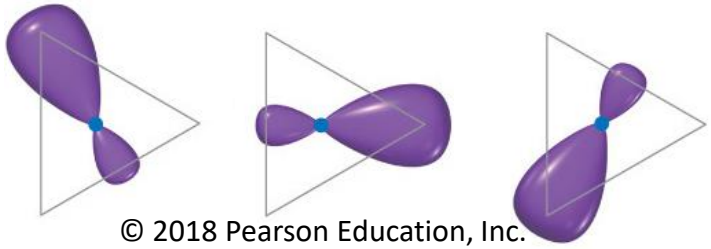




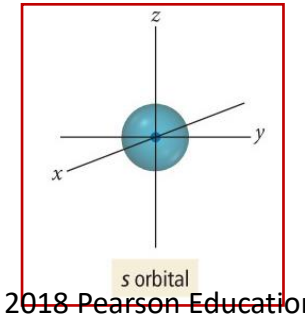
one unhybridized p-orbital

Energy ↑

hybridization →

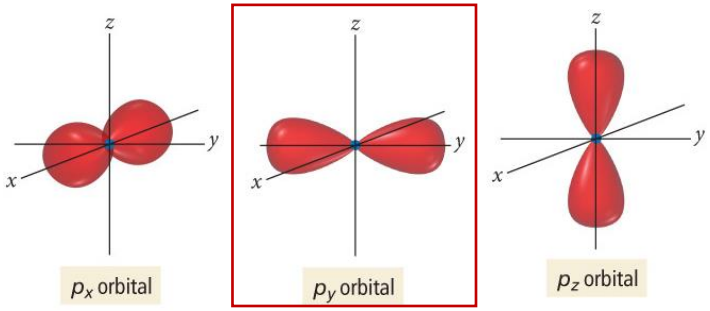


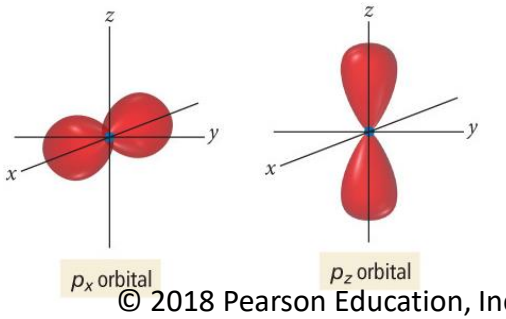
three new identical sp^2-orbitals



unhybridized **sp^2 hybridized**

Orbital Energies: Unhybridized vs. sp Hybridized



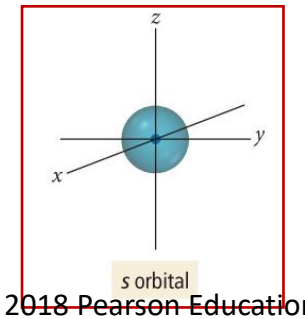


two unhybridized p-orbitals

Energy

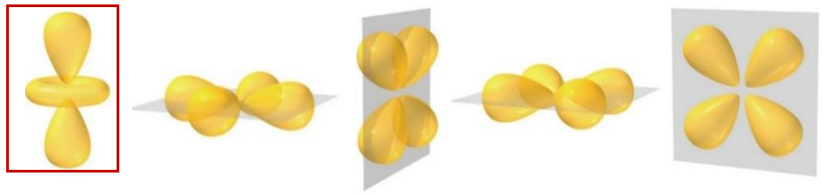
hybridization

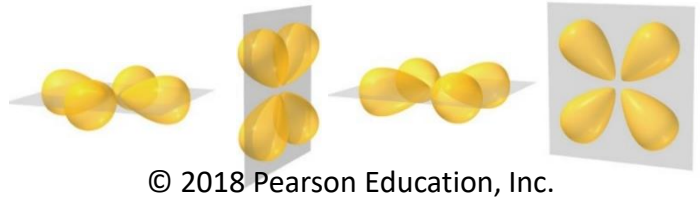
two new identical sp-orbitals



unhybridized **sp hybridized**

Orbital Energies: Unhybridized vs. sp^3d Hybridized

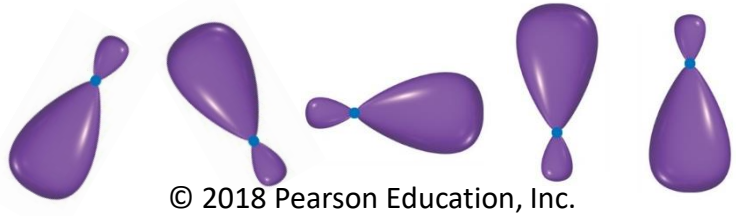




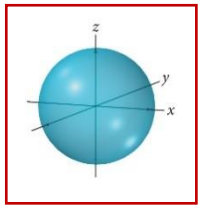
four unhybridized d-orbitals

Energy ↑

hybridization →



five new identical sp^3d-orbitals

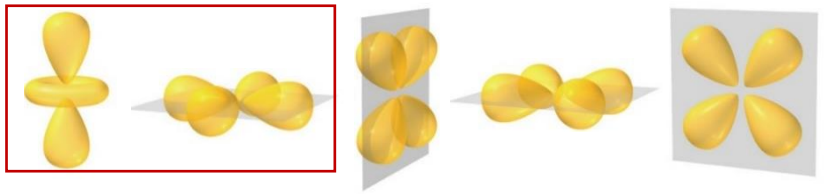


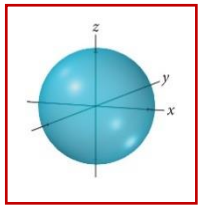
sp^3d hybrid orbitals (shown together)

unhybridized → **sp^3d hybridized**

Orbital Energies: Unhybridized vs. sp^3d^2 Hybridized

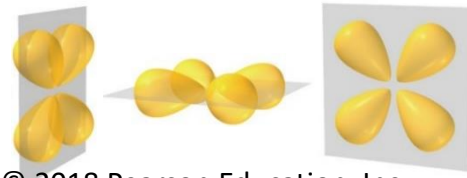
Energy ↑



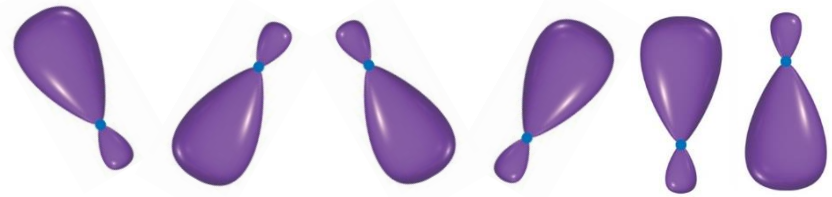


unhybridized

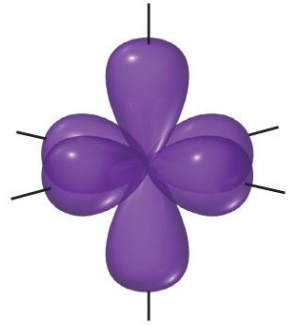
hybridization



three unhybridized d-orbitals



six new identical sp^3d^2-orbitals

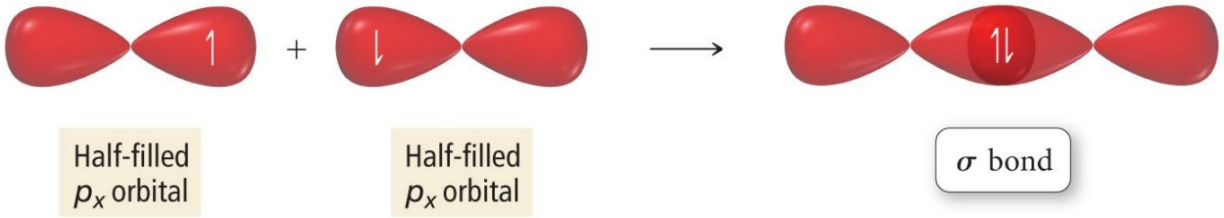


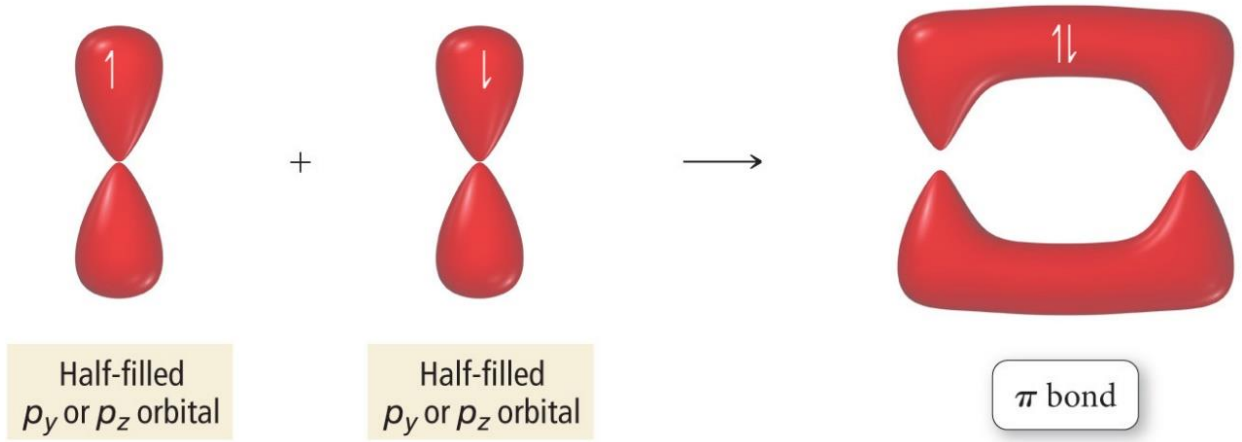
sp^3d^2 hybrid orbitals (shown together)

sp^3d^2 hybridized

Orbital Overlap: σ vs. π bonds

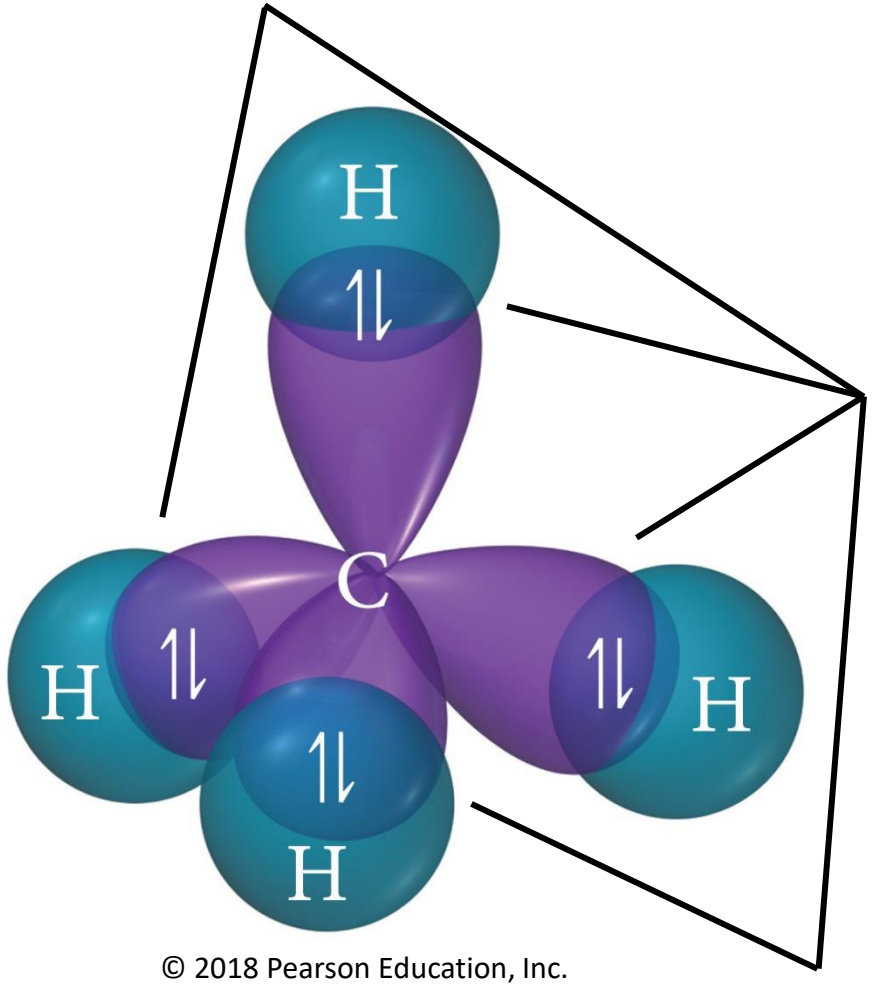
- sigma (σ) bonds
  - head-to-head overlap of two atomic orbitals
  - can be hybridized or unhybridized orbitals overlapping
  - free rotation around sigma bonds are possible
- pi (π) bonds
  - side-to-side overlap of two atomic orbitals
  - usually unhybridized and *parallel* p-orbitals overlapping
    - or d-orbitals on atoms with expanded octets
  - free rotation not possible due to pi bond
- for a given pair of atoms, a sigma bond is typically stronger than a pi bond
  - sigma bonds have greater orbital overlap than pi bonds
  - greater orbital overlap = stronger bond





Bonding Scheme of Methane (CH_4)

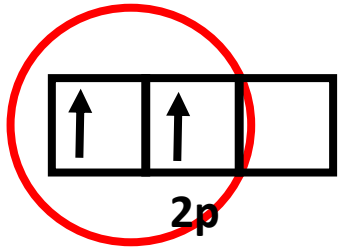
bonding scheme = identifies the orbitals overlapping to form bonds within a molecule and specifies the types of bonds (σ vs. π)



Each C–H bond is
σ: C(sp^3) – H($1s$)

Hybridization and σ-bonds in methane (CH_4)

only 2 half-filled orbitals
available for bond-making



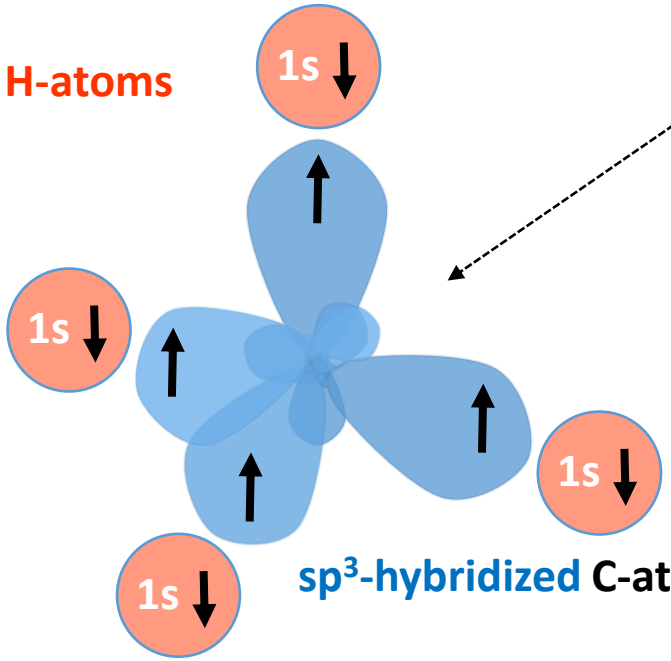
valence-orbital diagram for unhybridized C-atom
4 valence electrons

sp^3 hybridization

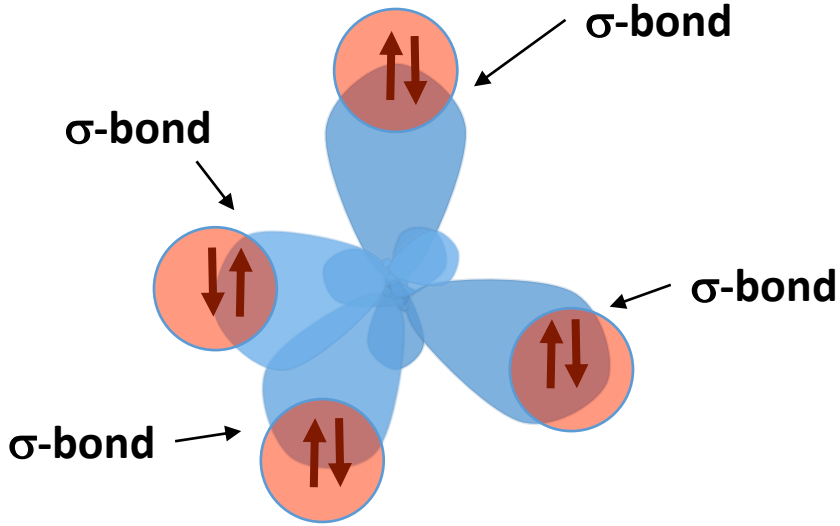
now there are 4 half-filled orbitals
available for (sigma) bond-making

valence-orbital diagram for sp^3-hybridized C-atom
4 valence electrons

4 unhybridized H-atoms

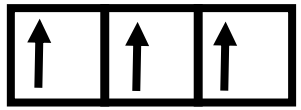


form C–H bonds



CH_4 with four sigma-bonds

Hybridization and σ-bonds in ammonia (NH_3)



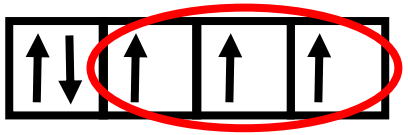
2p

2s

valence-orbital diagram for unhybridized N-atom
5 valence electrons

sp^3 hybridization

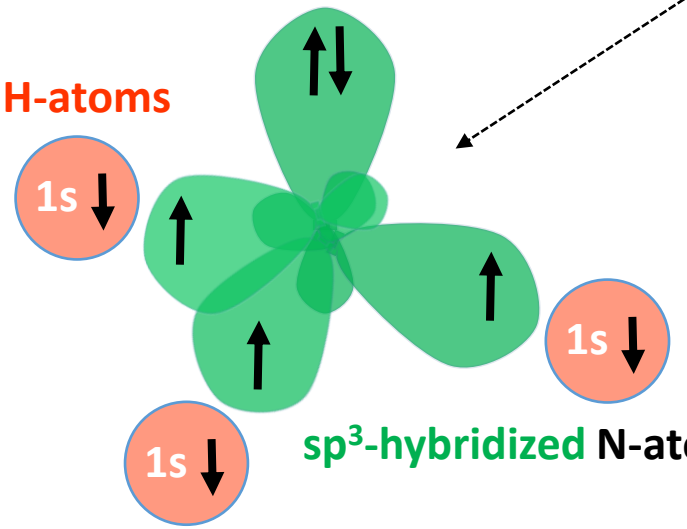
3 half-filled orbitals available for (sigma) bond-making



sp^3

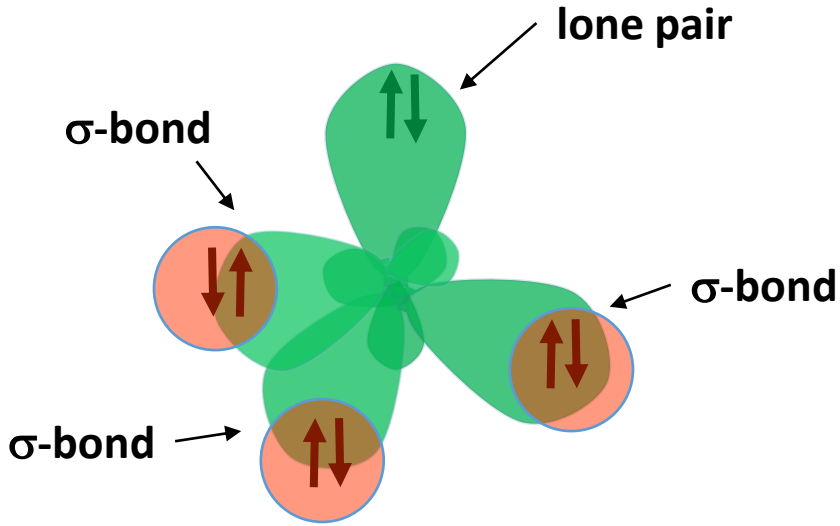
valence-orbital diagram for sp^3-hybridized N-atom
5 valence electrons

3 unhybridized H-atoms



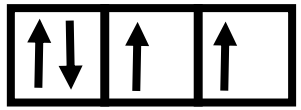
sp^3-hybridized N-atom

form N–H bonds



NH_3 with three sigma-bonds

Hybridization and σ-bonds in water (H_2O)



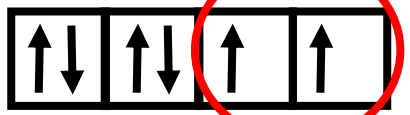
2p

2s

valence-orbital diagram for unhybridized O-atom
6 valence electrons

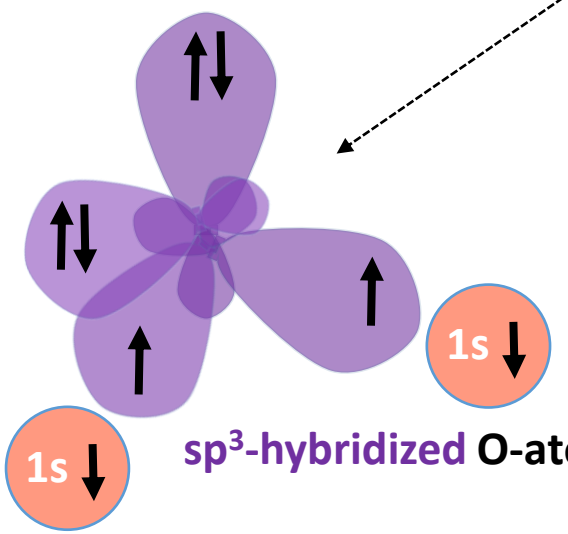
sp^3 hybridization

2 half-filled orbitals available for (sigma) bond-making



sp^3

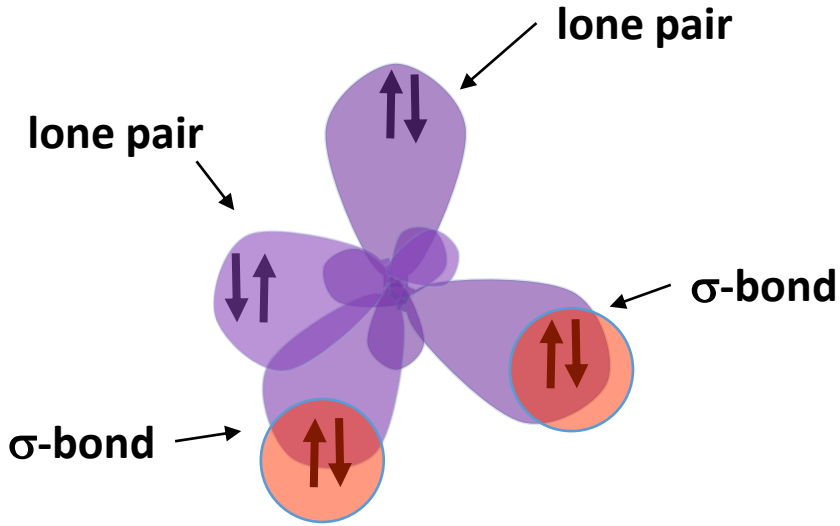
valence-orbital diagram for sp^3-hybridized O-atom
6 valence electrons



2 unhybridized H-atoms

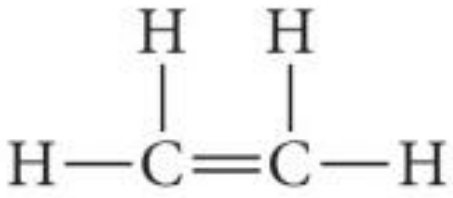
sp^3-hybridized O-atom

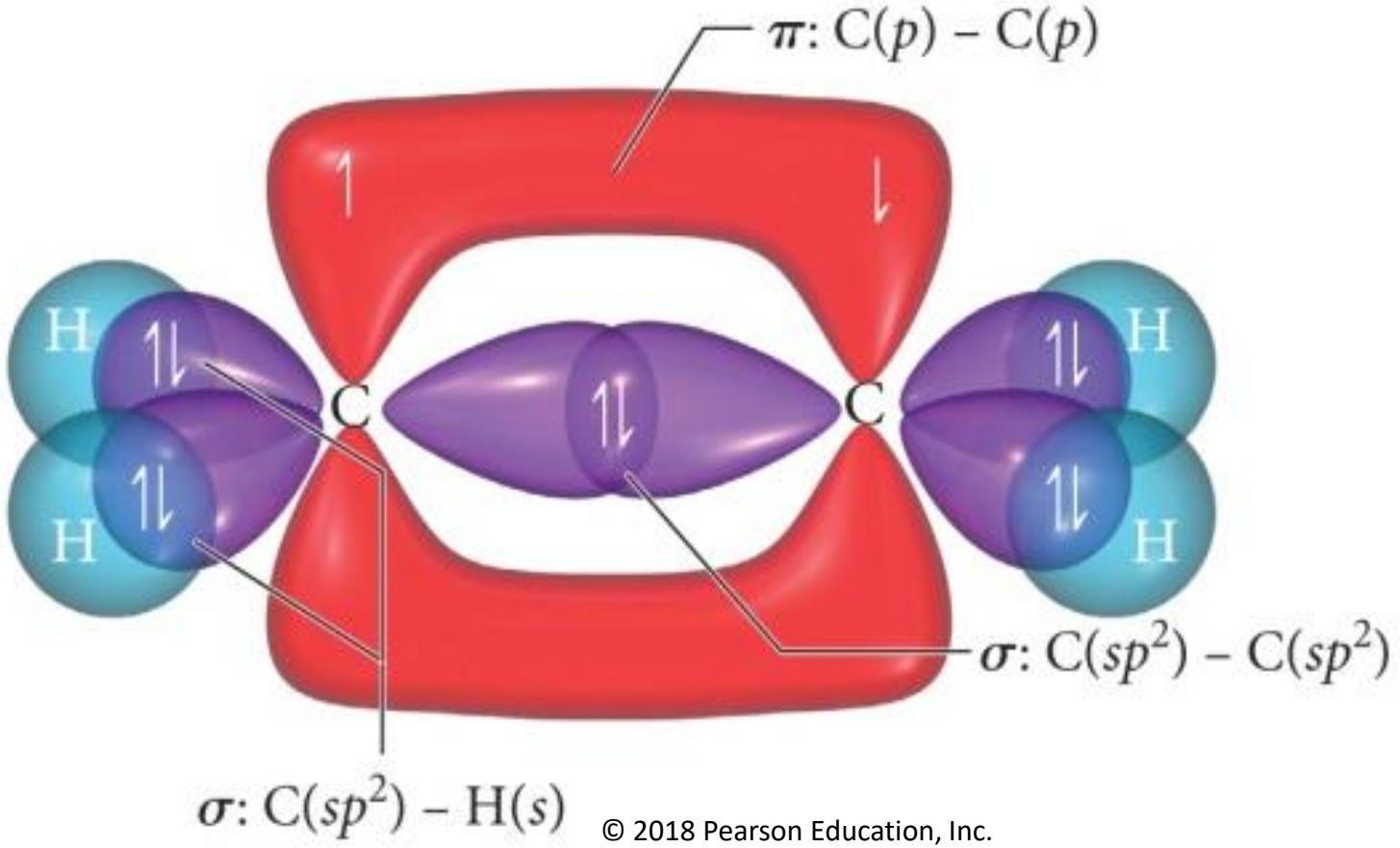
form O–H bonds



H_2O with two sigma-bonds

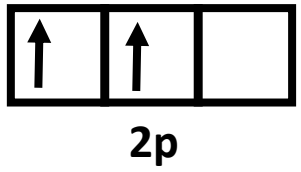
Bonding Scheme of Ethene (C_2H_4)





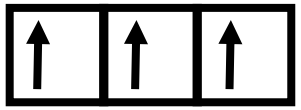
hindered rotation due to π bond
may lead to cis-trans isomerism

Hybridization, σ-bonds and π-bond in ethene (C_2H_4)



valence-orbital diagram for unhybridized C-atom

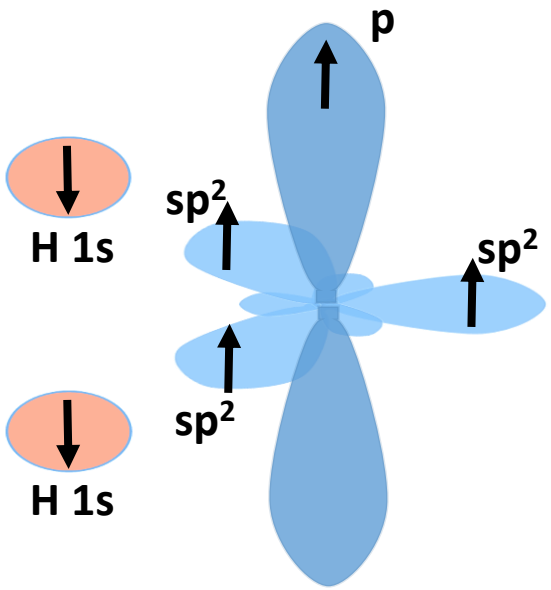
sp^2 hybridization



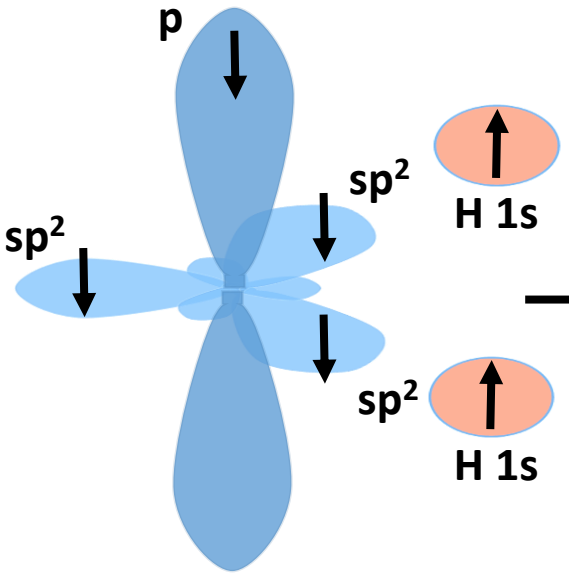
1 half-filled unhybridized p-orbital for π-bond

3 half-filled hybrid orbitals for σ-bonds

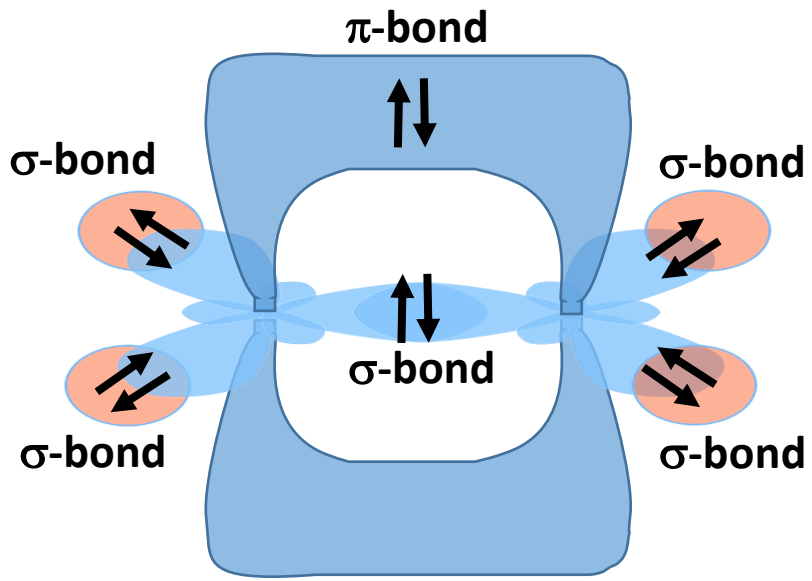
valence-orbital diagram for sp^2-hybridized C-atom



sp^2-hybridized C-atom

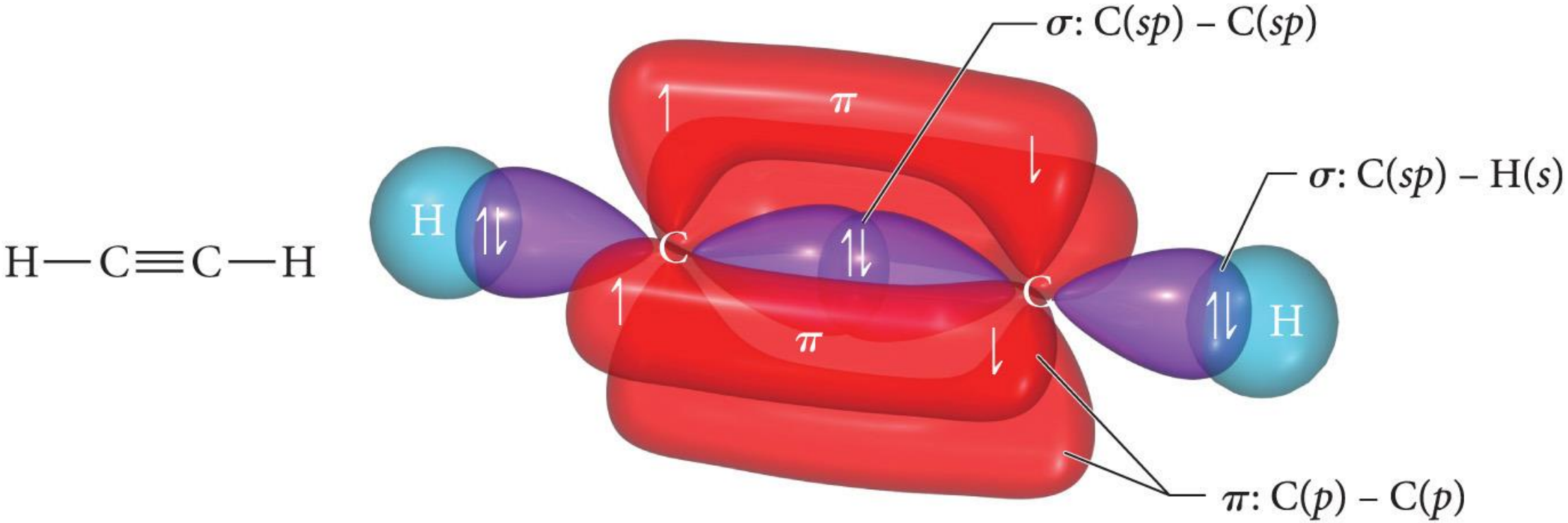


sp^2-hybridized C-atom

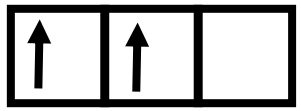


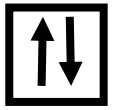
C_2H_4 with five sigma-bonds and one pi-bond

Bonding Scheme of Ethyne (C_2H_2)



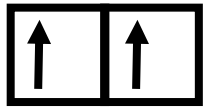
Hybridization, σ-bonds and π-bonds in ethyne (C_2H_2)





valence-orbital diagram for unhybridized C-atom

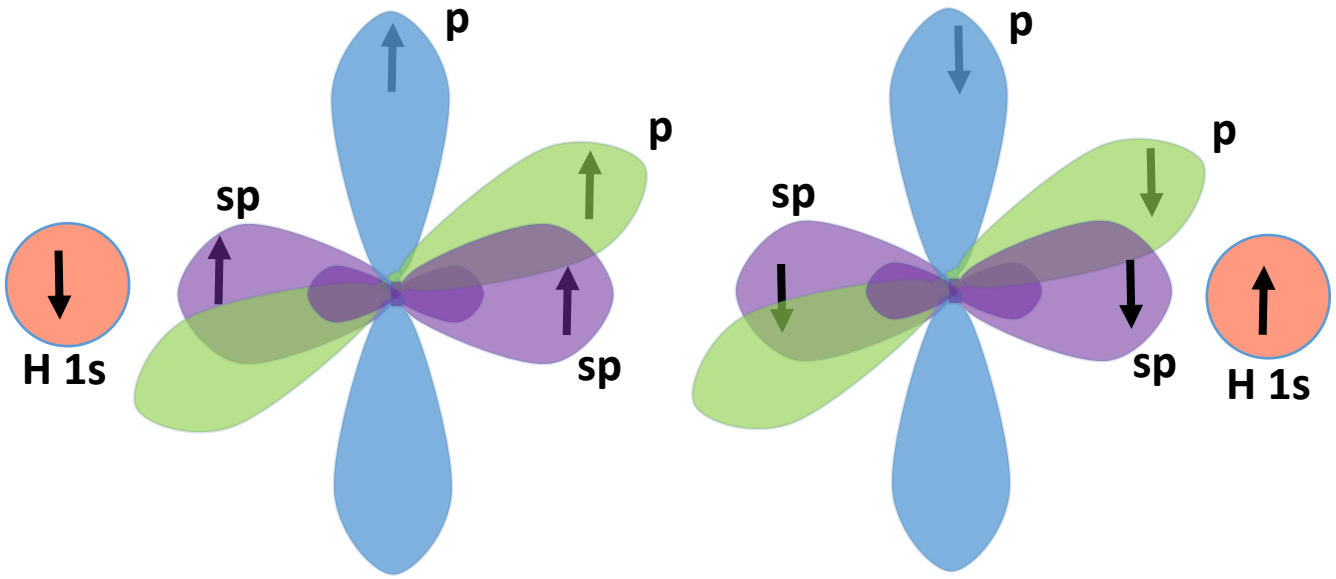
sp hybridization



2 half-filled hybrid orbitals for σ-bonds

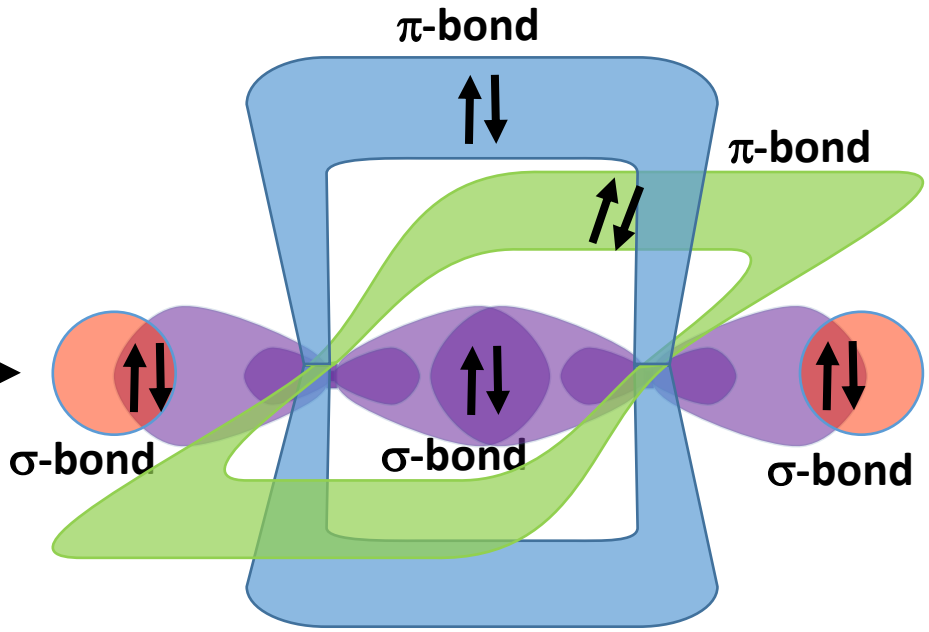
2 half-filled unhybridized p-orbitals for π-bonds

valence-orbital diagram for sp-hybridized C-atom



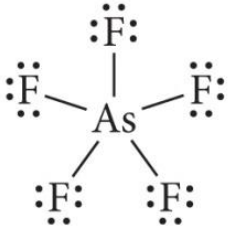
sp-hybridized C-atom

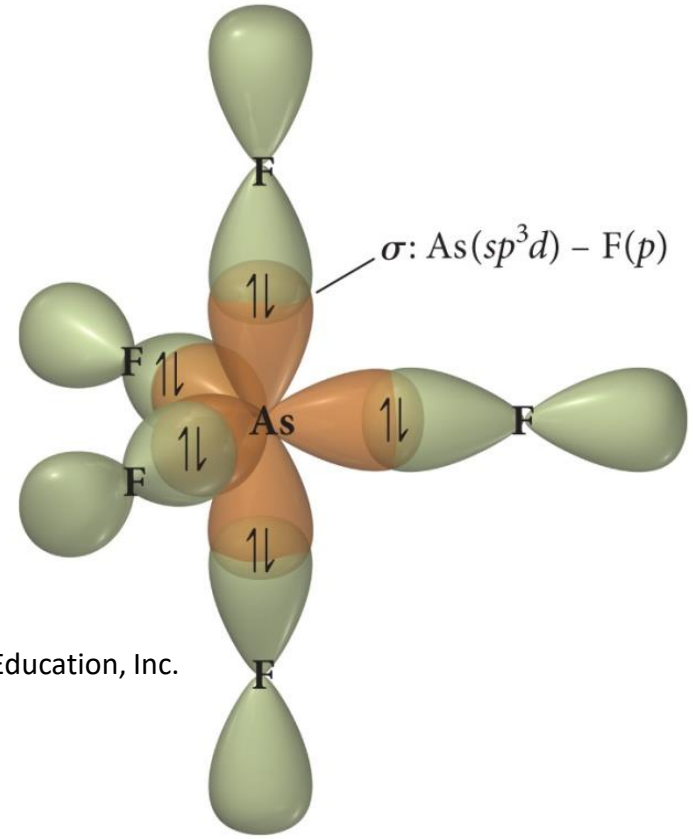
sp-hybridized C-atom

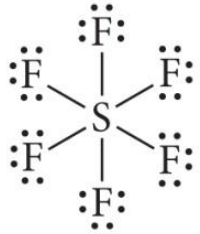


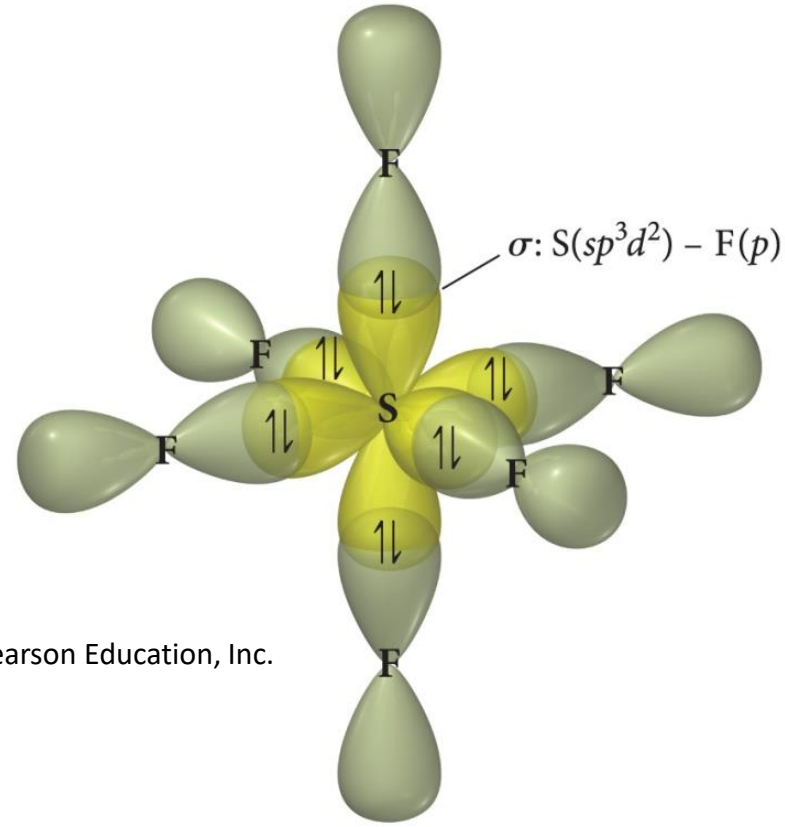
C_2H_2 with three sigma-bonds and two pi-bonds

Bonding Schemes of AsF_5 and SF_6









Practical skills related to hybridization and valence bond theory

- you should be able to determine the hybridization of all interior atoms of a compound given the compound's name, formula, or Lewis structure
  - for example, give the hybridization of all interior atoms of acetic acid (CH_3COOH)

- you should be able to determine the number of sigma bonds and pi bonds in a given compound
  - for example, how many sigma bonds and pi bonds are in carbon monoxide?

- you should be able to write the bonding scheme for a molecule
  - for example, write the bonding scheme for HCN