Week Oct 28 – Nov 1

What will you be learning?

Bonding in Molecules with Resonance
What makes some materials conducting?
How do molecules interact with each other?

Learning Objectives this week:

- **Combination of valence bond theory, hybridization, and MO theory to explain resonance.**
- **How to count the number of orbitals in sigma and pi bond formation in a resonance structure?**
- **How do orbital combinations lead to the formation a band?**
- **What are valence and conduction bands, and how do we explain conductivity?**
- **What are intermolecular forces of interactions?**
- **How do we use these intermolecular forces of interactions to explain properties of molecules?**

McGill

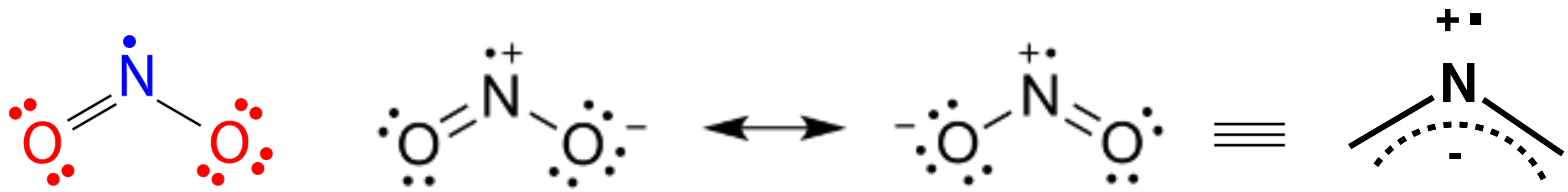
Resonance

NO_2

N $2s^2\ 2p^3$

O $2s^2\ 2p^4$

Total number of electrons based on valence shell electrons = 5 + 6(2) = 17



Resonance Structures:

More than one possible Lewis structure

Both structures for NO_2 are probable/plausible Lewis structures

Only electrons move (movement of lone pairs or multiple bonds)

Atoms **do not** move

Using a mix of valence bond theory, hybridization and MO theory we can help explain (and simplify) bonding in such molecules with resonance.

Resonance

NO_2

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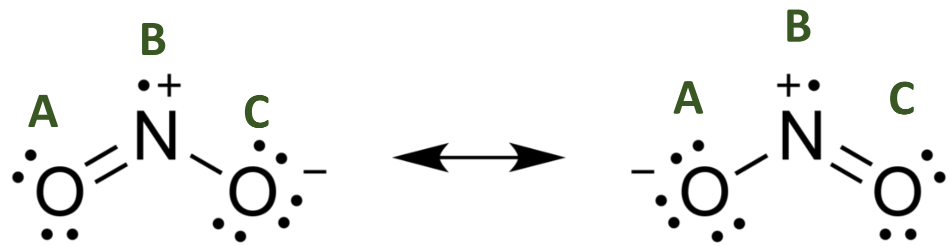
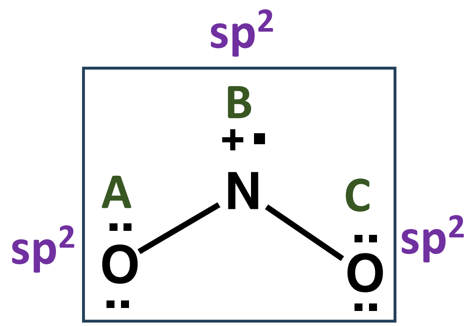


Stationary Structure

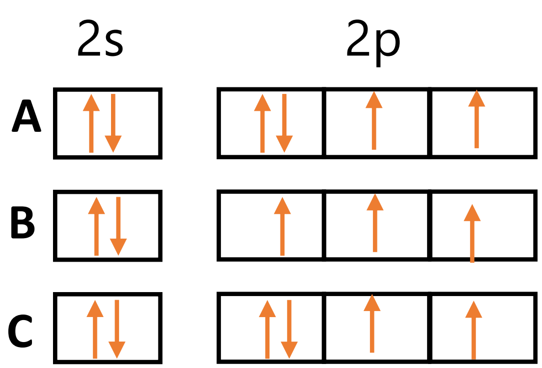


N $2s^2$ $2p^3$

O $2s^2$ $2p^4$

(valence orbitals)

Determine hybridization at each atom center



Number of electron groups = 3 = number of hybrid orbitals = 3 = sp^2

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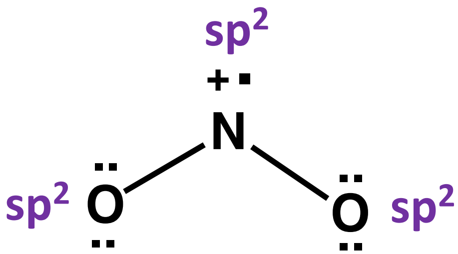
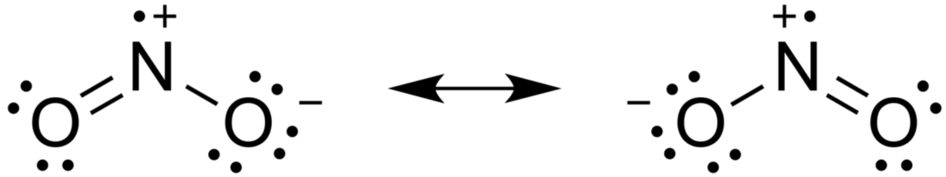
Resonance

Using a mix of valence bond theory and MO theory we can help explain (and simplify) bonding in such molecules with resonance.





N $2s^2$ $2p^3$

O $2s^2$ $2p^4$

(valence orbitals)

Each oxygen has ___**4**___ valence orbitals

Nitrogen has ___**4**___ valence orbitals

In NO_2, total ___**12**___ valence orbitals

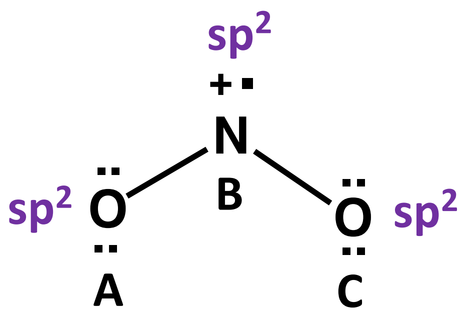
Total orbitals = 12

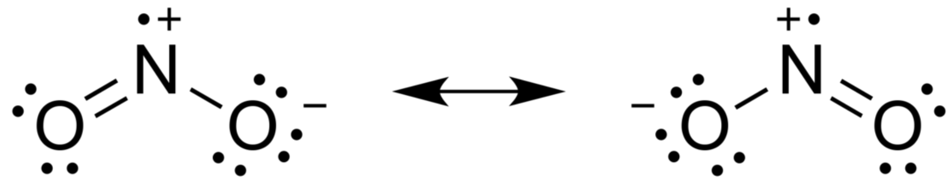
Hybrid orbitals = 9

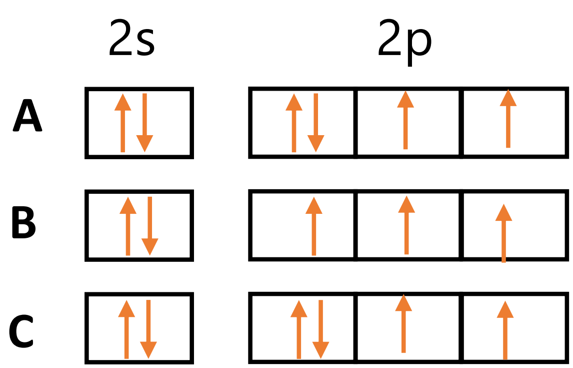
Unhybridized orbitals = 12 – 9 = 3

For all the sigma bonds we use valence bond theory and hybridization
- the central nitrogen is sp^2 hybridized (in either structure)
- One sigma bond each with the two terminal oxygen atoms
- Third sp^2 orbital contains the lone electron on the central atom

NO_2 : delocalized π electrons







Still remaining:
Atoms A, B and C are left with one unhybridized p orbital each.

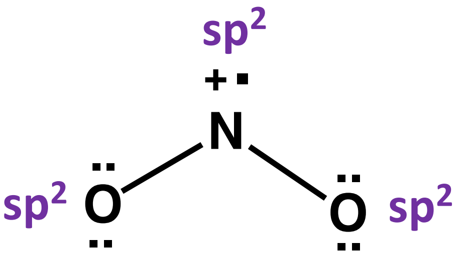
Total = 3

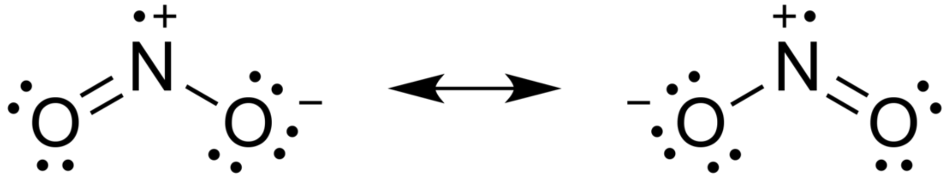
Delocalized electron count (moving parts):

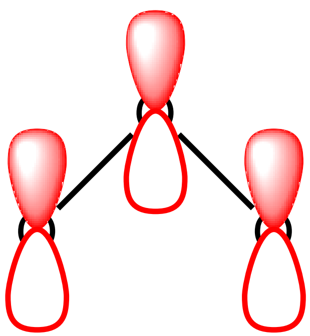
For the stationary structure, we removed moving bond (one that was making a double bond on either side) and a moving lone pair of electrons.

These four electrons are delocalized in the structure.

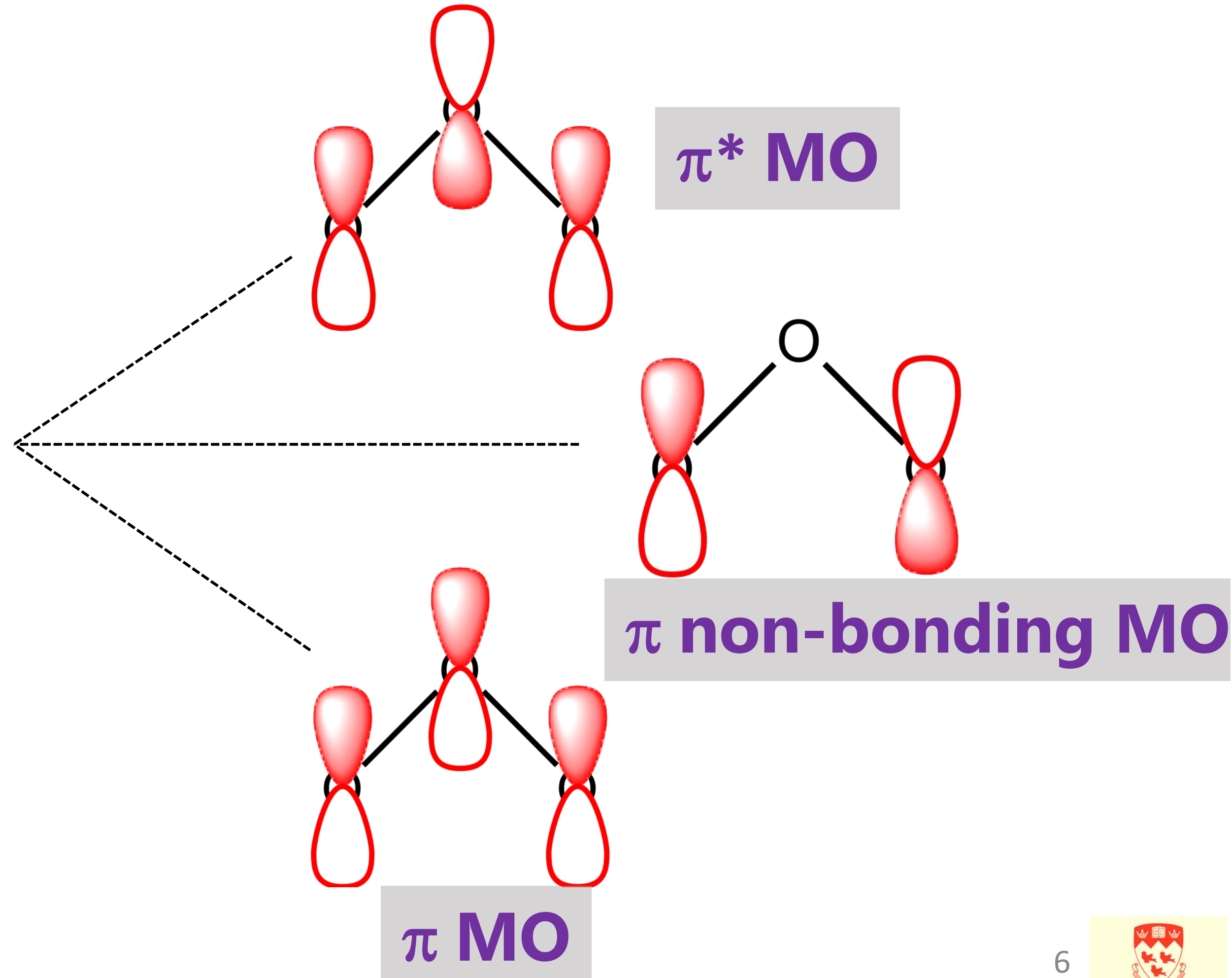
NO_2 : delocalized π electrons



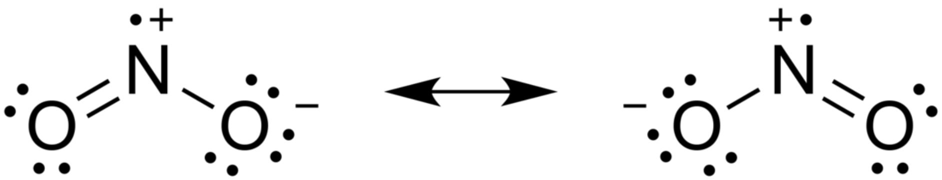




From LCAO of 3 p orbitals

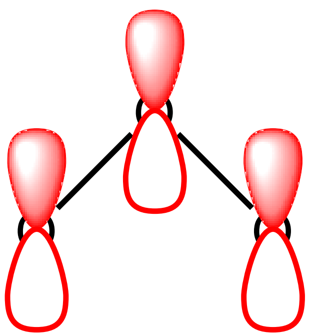


NO_2 : delocalized π electrons



3 unhybridized p orbitals

4 electrons



From LCAO of 3 p orbitals

π* MO

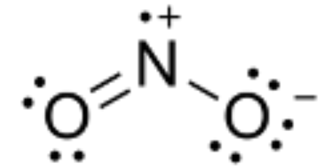
π non-bonding MO

π MO

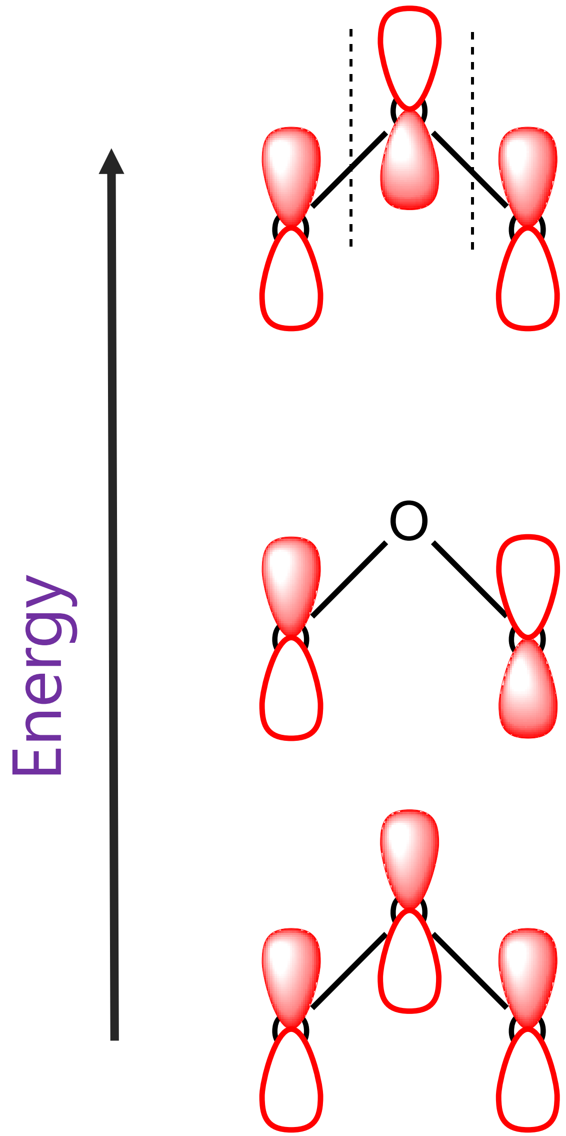
3 π MOs

NO_2 : delocalized π electrons

For hybridization, we removed moving bond (one that was making a double bond on either side) and a moving lone pair of electrons.



These four electrons are delocalized in the structure.

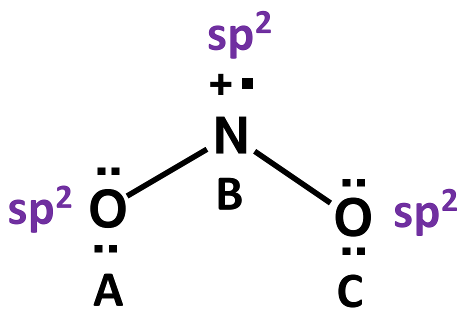


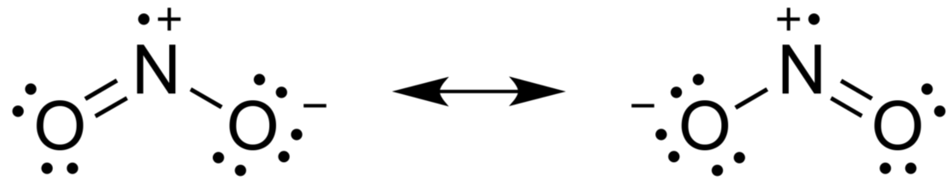
π* MO

π non-bonding MO ↑↓

π MO ↑↓

Bonding in NO_2: Resonance structure





Break down the structure into two parts:
Stationary atoms and bonds
Moving bonds and any lone pair of electrons.

Consider the stationary structure and determine hybridization at each atom center.

Note the remaining p orbitals at each atom center that are unhybridized.

Use hybridization to explain the formation of sigma bonds using valence bond theory.

In NO_2, central nitrogen atoms forms two sp^2-sp^2 sigma bonds.

Use the remaining p orbitals at each atom center for combination using MO theory.

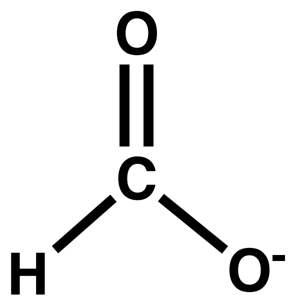
Number of p orbitals combined should be equal to number of π MOs formed.

In NO_2 we combined three p orbitals (one at each atom) to form three delocalized π orbitals.

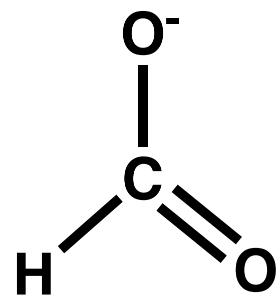
Place your moving electrons into MOs.

Practice Question 1

What is the relationship between the two structures (A and B) given below?
Based on the structures shown below:
How many pi molecular orbitals are in the molecule?
How many electrons are delocalized in the molecule?



Structure A



Structure B

Practice Question 1

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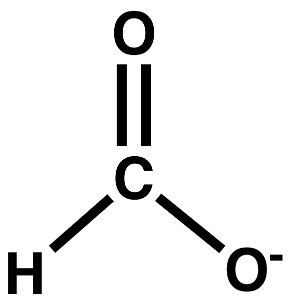

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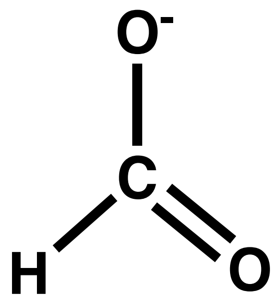
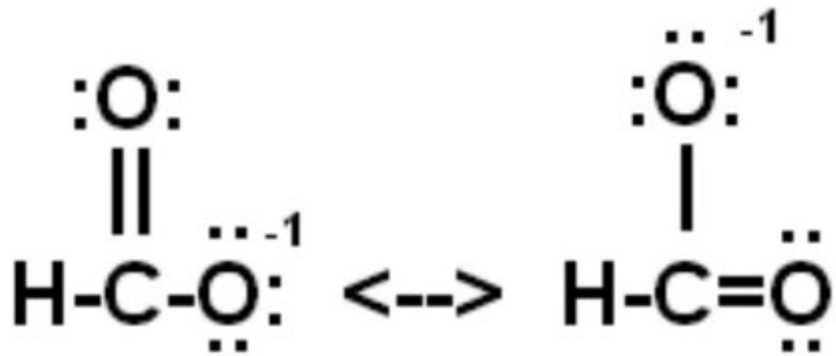


Structure B



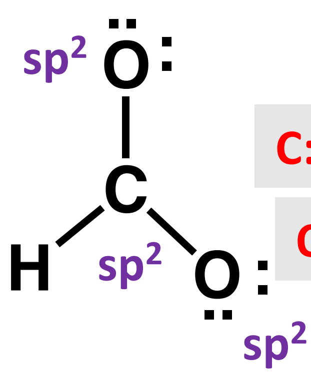
Structure A and B are Resonance structures – the electrons are delocalized but the atoms and sigma bonds remain the same.

Atoms are stationary, but one bond and one lone pair of electrons and charge are moving.

H $1s^1$

C $2s^2\ 2p^2$

O $2s^2\ 2p^4$



Stationary structure

C: Number of electron groups = 3 = number of hybrid orbitals = 3 = sp^2

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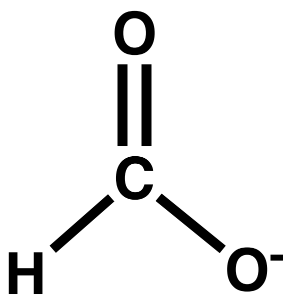

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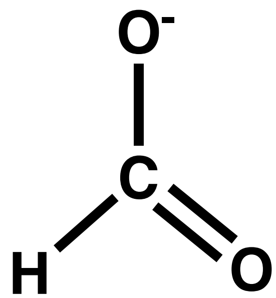
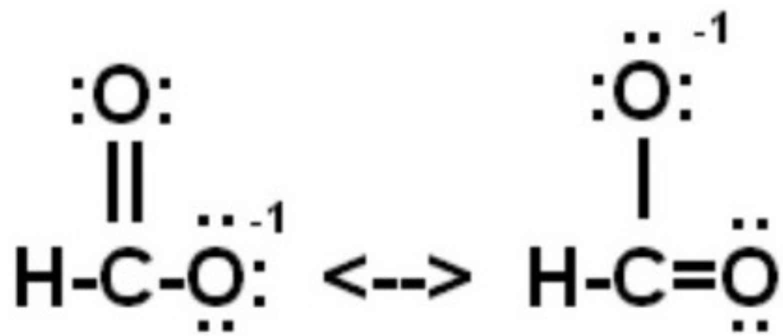


Structure B



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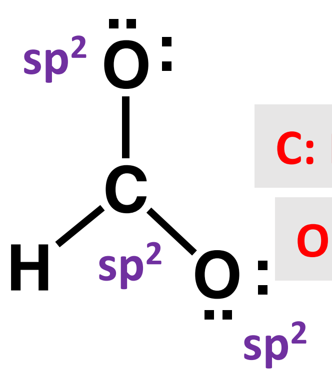

Stationary structure

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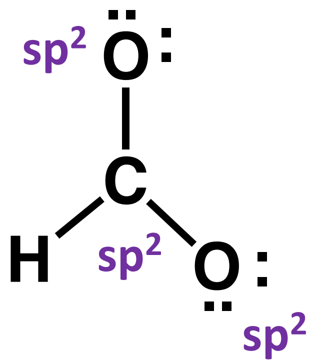
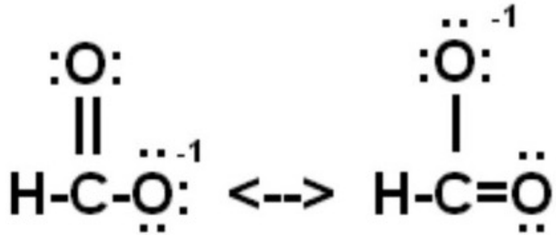
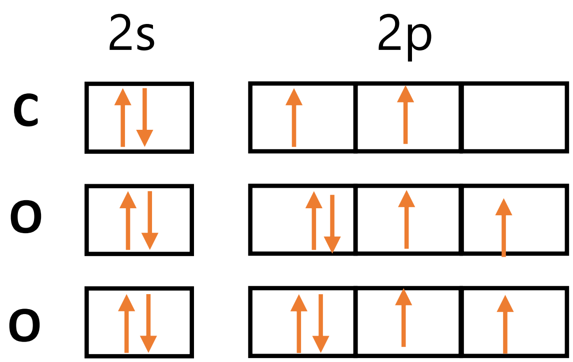
C forms two sp^2-sp^2 σ bonds with two O atoms and one sp^2-s σ bond with hydrogen.

$[HCO_2]^-$: delocalized π electrons







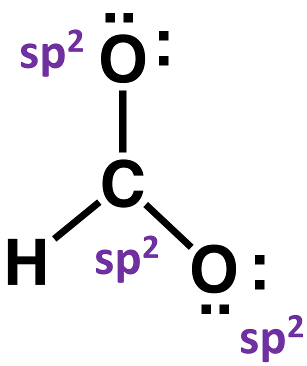
Still remaining:
Carbon and two oxygen atoms are left with one unhybridized p orbital each.

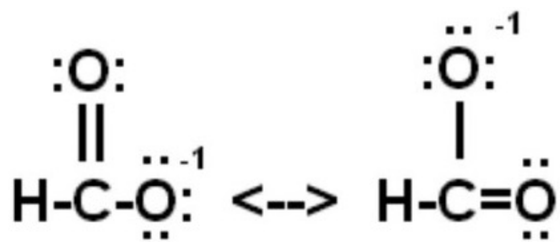
Total = 3

For hybridization, we removed moving bond (one that was making a double bond on either side) and a moving lone pair of electrons.

These four electrons are delocalized in the structure.

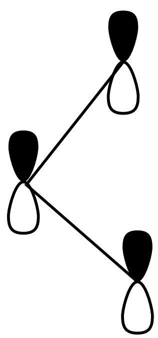
$[HCO_2]^-$: delocalized π electrons





3 unhybridized p orbitals

4 electrons



From LCAO of 3 p orbitals

π* MO

π non-bonding MO

π MO

3 π MOs

$[HCO_2]^-$: delocalized π electrons

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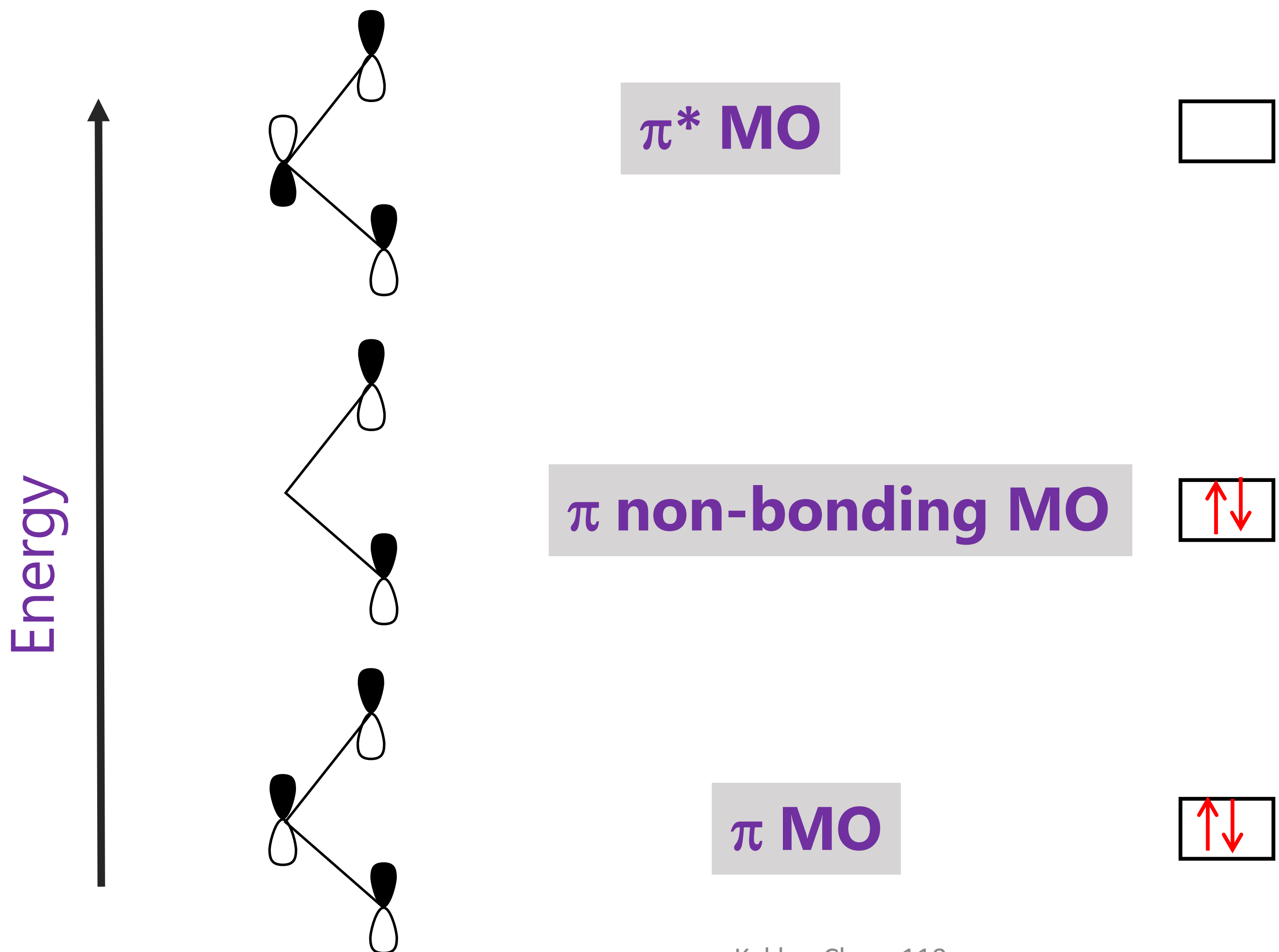

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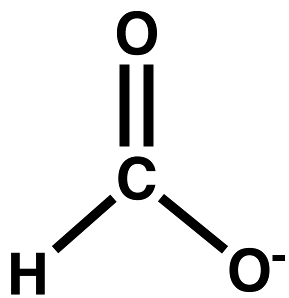
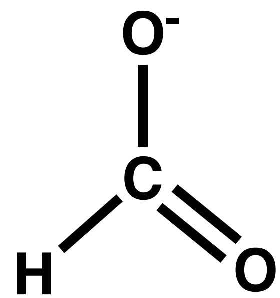


Structure A



Structure B

Practice Question 1

Based on the structures shown below:
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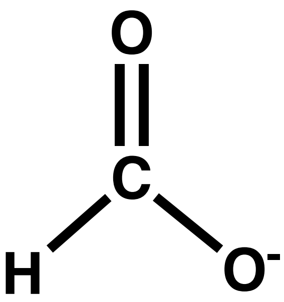
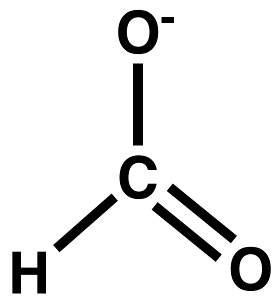
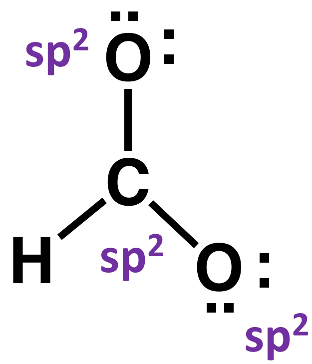
How many electrons are delocalized in the molecule?

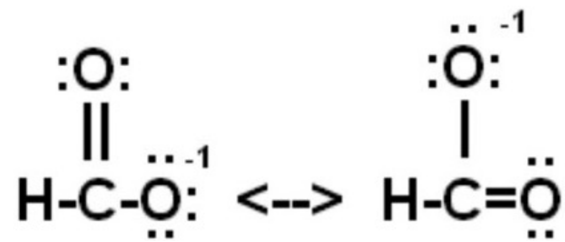


Structure A



Structure B





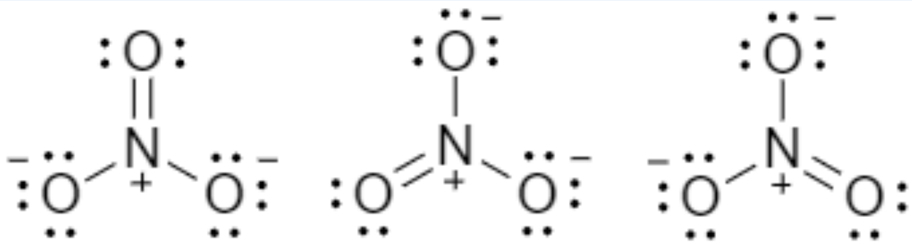
Structure A and B are Resonance structures – the electrons are delocalized but the atoms and sigma bonds remain the same.

There are 3 unhybridized p orbitals (carbon and 2 oxygens are all sp^2 hybridized) and hence 3 π molecular orbitals.

There are 4 total delocalized electrons.
2 in the π bond, and a lone pair that is delocalized on the two oxygen atoms.

Bonding in NO_3^-: Resonance structure

NO_3^-

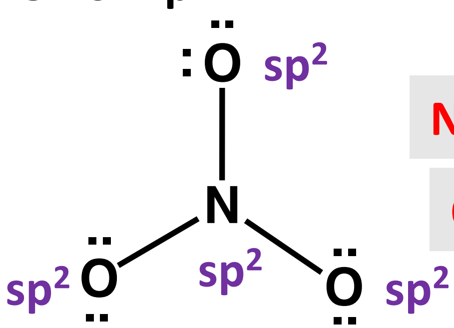


There are three resonance structures – the electrons are delocalized but the atoms and sigma bonds remain the same.

Atoms are stationary, but one bond and lone pair of electrons and charge are moving.

N $2s^2\ 2p^3$

O $2s^2\ 2p^4$



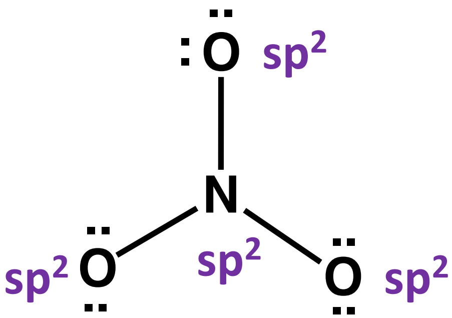
Stationary structure

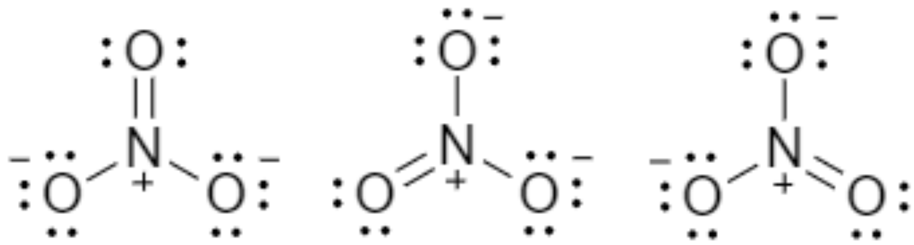
N: Number of electron groups = 3 = number of hybrid orbitals = 3 = sp^2

O: Number of electron groups = 3 = number of hybrid orbitals = 3 = sp^2

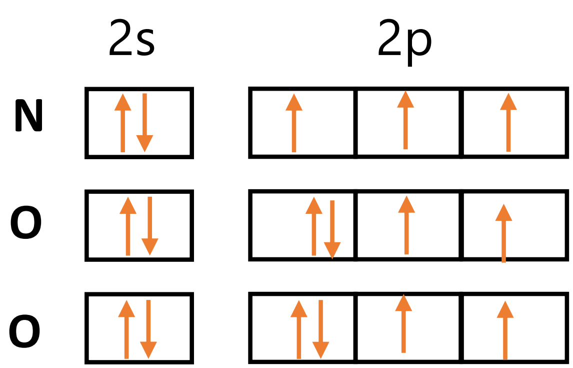
N forms three sp^2-sp^2 σ bonds with three O atoms

$[NO_3]^-$: delocalized π electrons





1 2 3



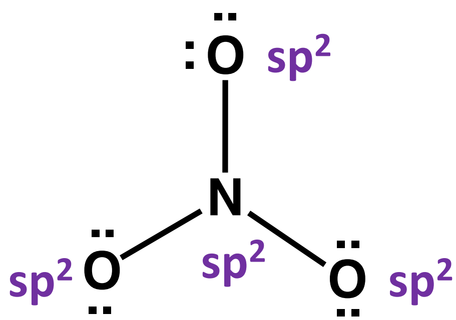
Still remaining:
Nitrogen and three oxygen atoms are left with one unhybridized p orbital each.

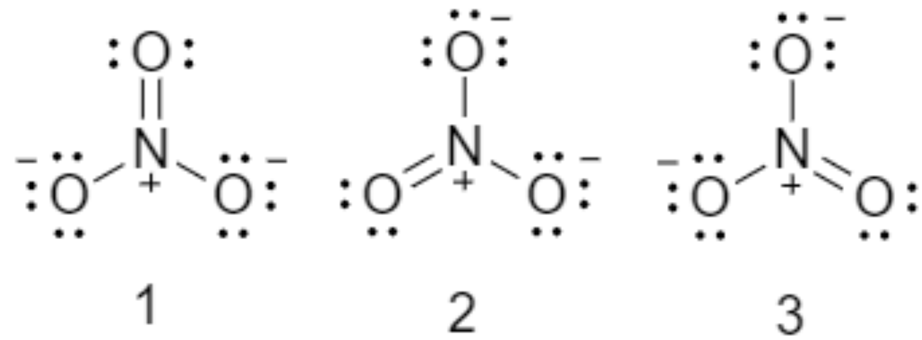
Total = 4

For hybridization, we removed moving bond (one that was making a double) and moving lone pairs of electrons. Total number of electrons = 6.

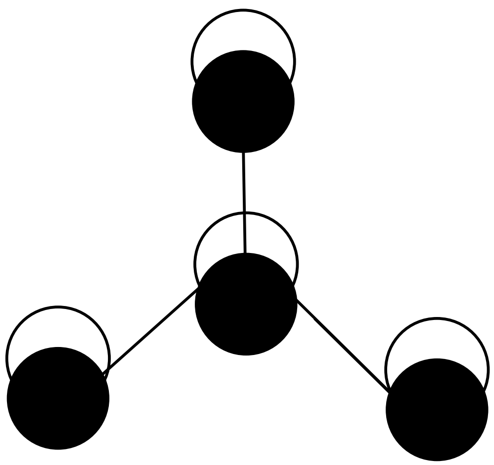
These six electrons are delocalized in the structure.

$[NO_3]^-$: delocalized π electrons

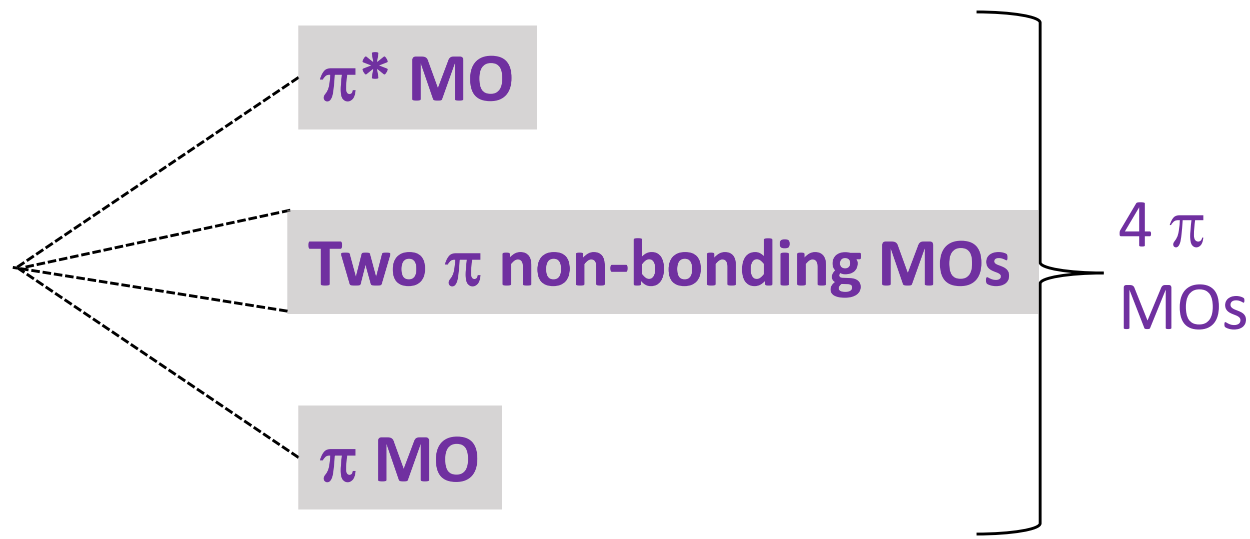




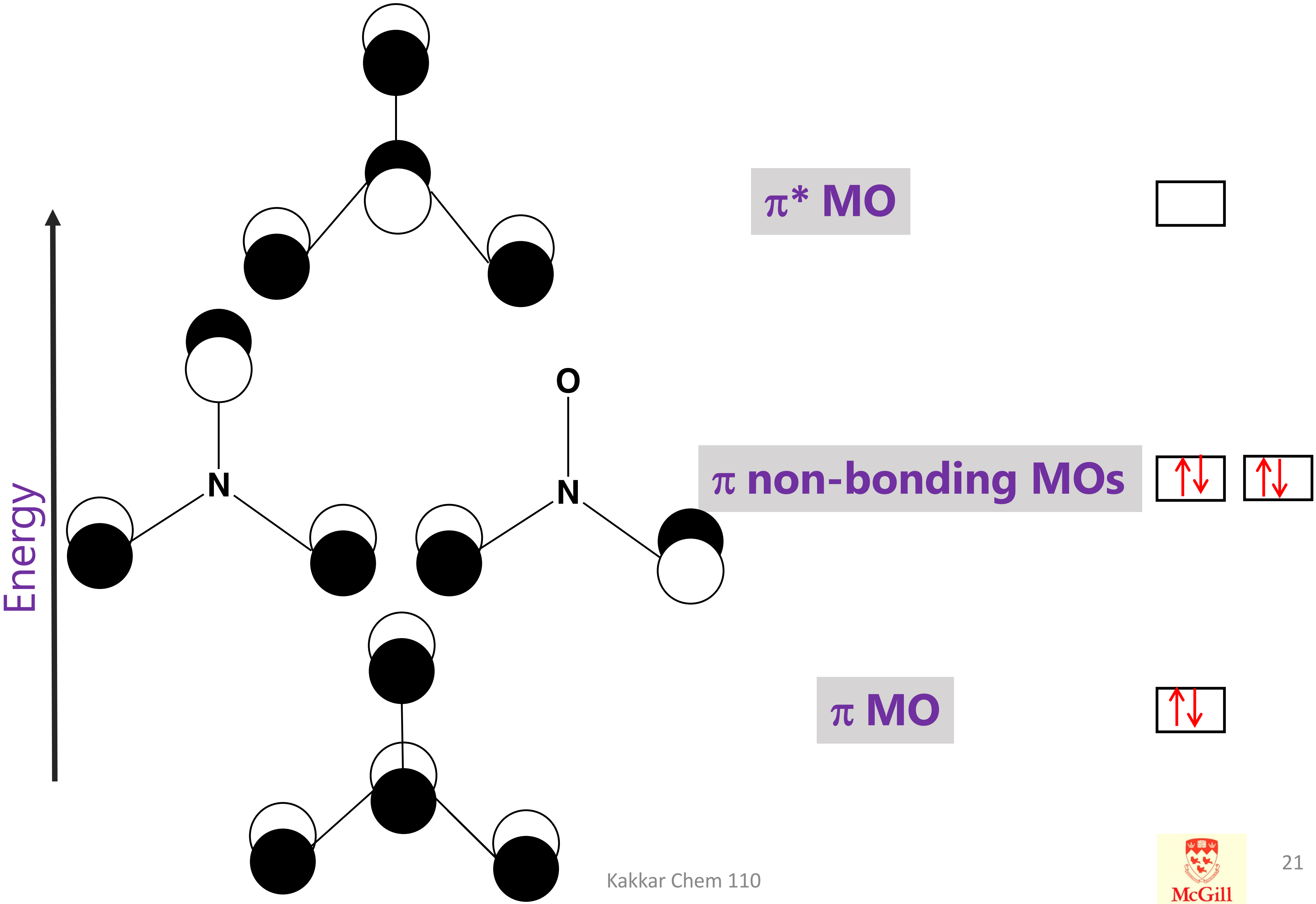
4 unhybridized p orbitals



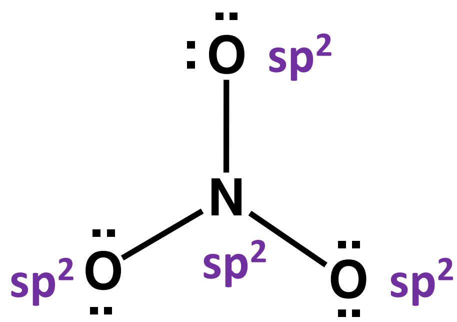
From LCAO of 4 p orbitals

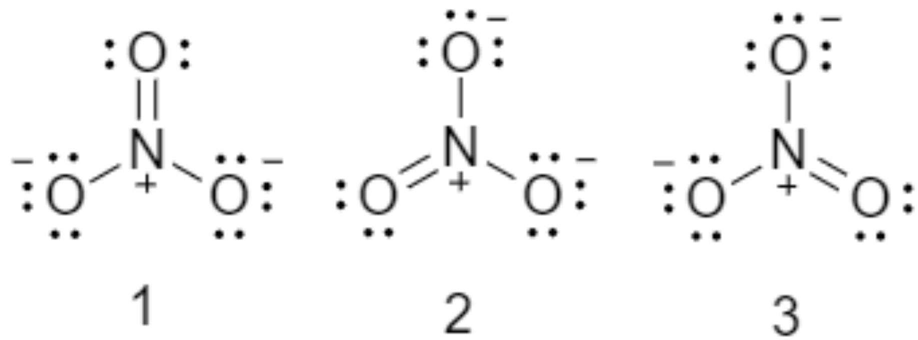


$[NO_3]^-$: delocalized π electrons



Bonding in NO_3^-: Resonance structure

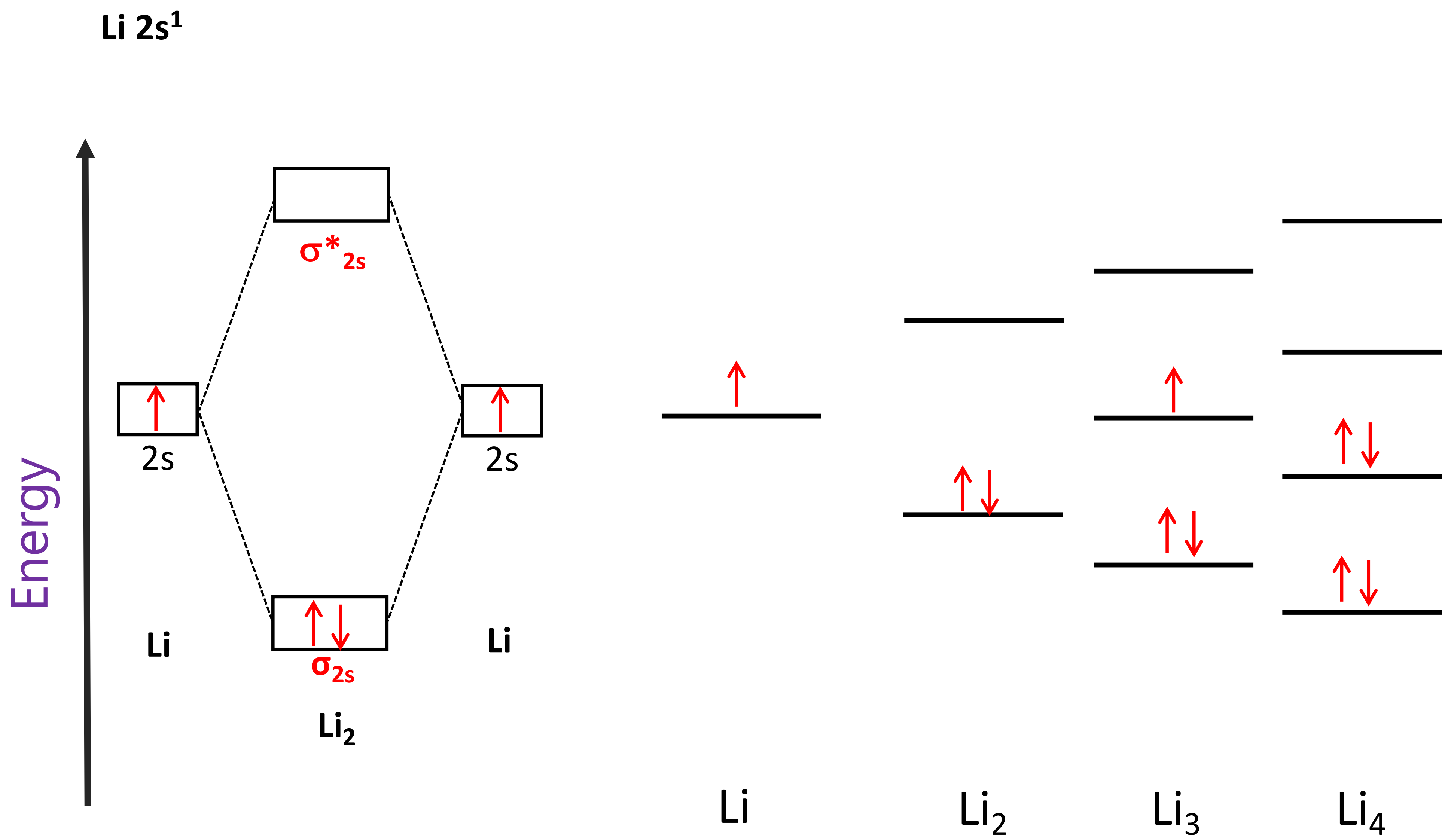




There are 4 unhybridized p orbitals (nitrogen and 2 oxygens are all sp^2 hybridized) and hence 4 π molecular orbitals.

There are 6 total delocalized electrons.
2 in the π bond, and lone pairs that are delocalized on the oxygen atoms.

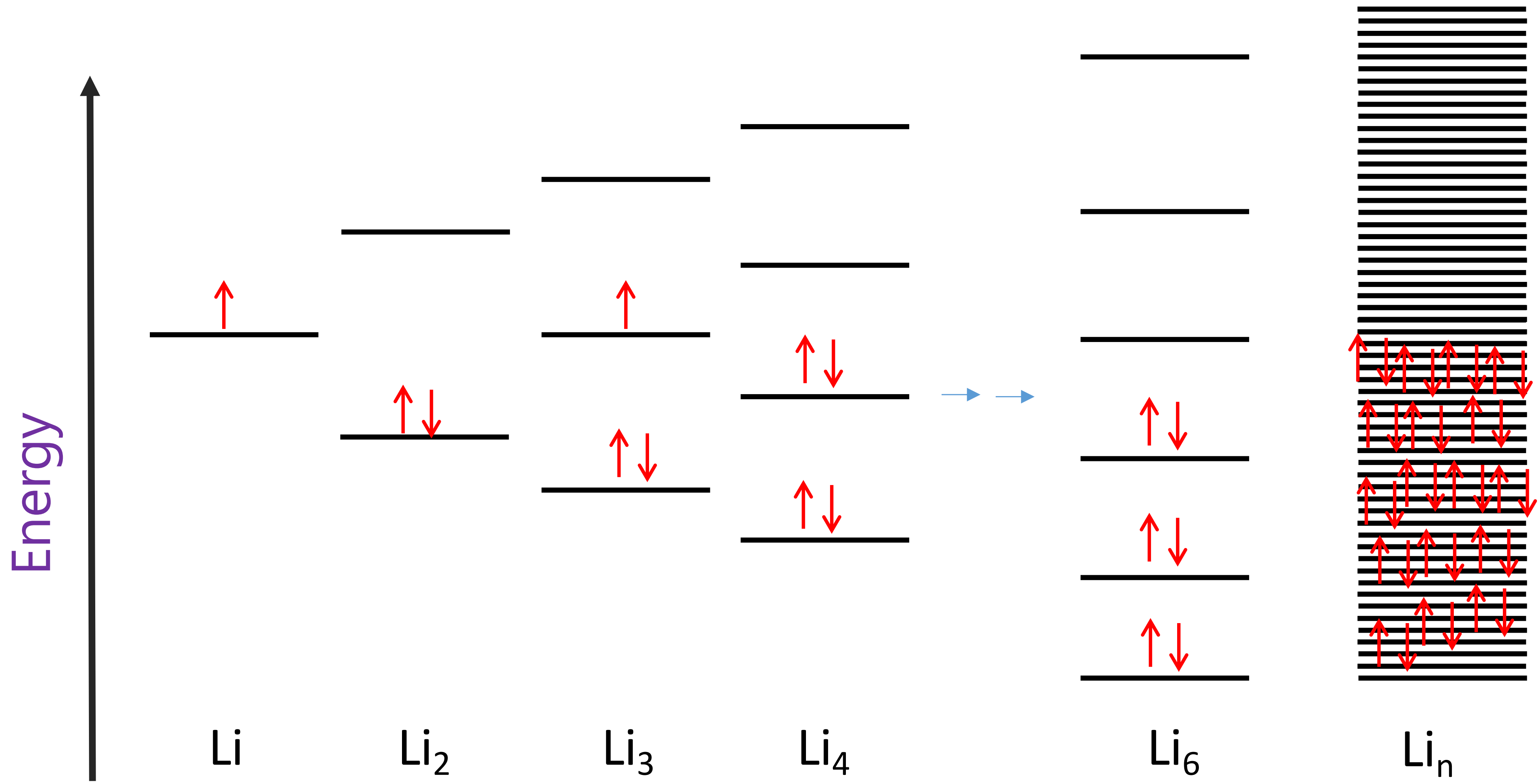
Band Theory: Group 1 Metals



Band Theory: Group 1 Metals

Li $2s^1$

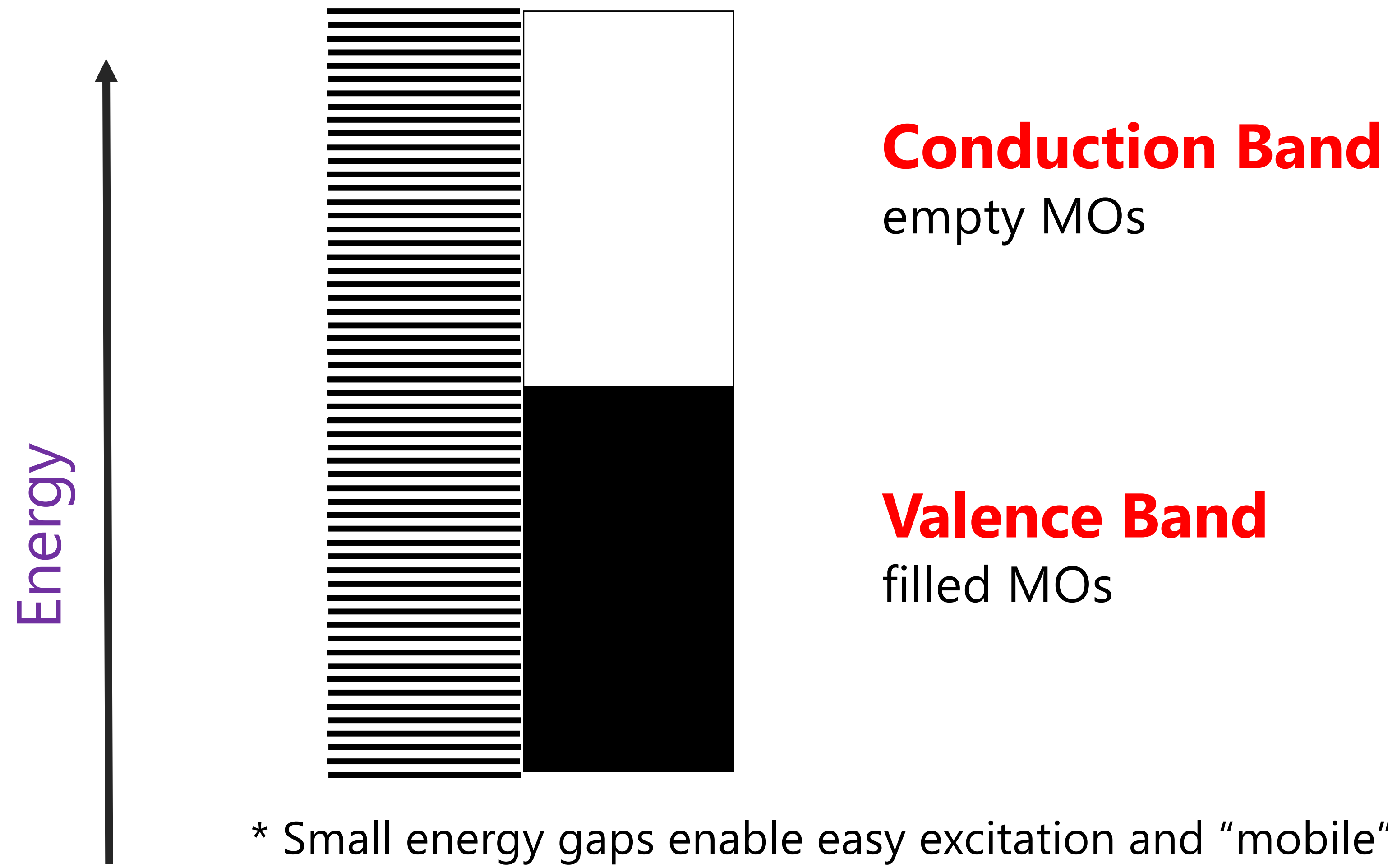
Li_n (metal): ***n*** 2s AOs = ***n*** MOs (***n*** valence electrons)



Li 2s Energy Band

Li $2s^1$

Li_n (metal): ***n*** 2s AOs = ***n*** MOs (***n*** valence electrons)

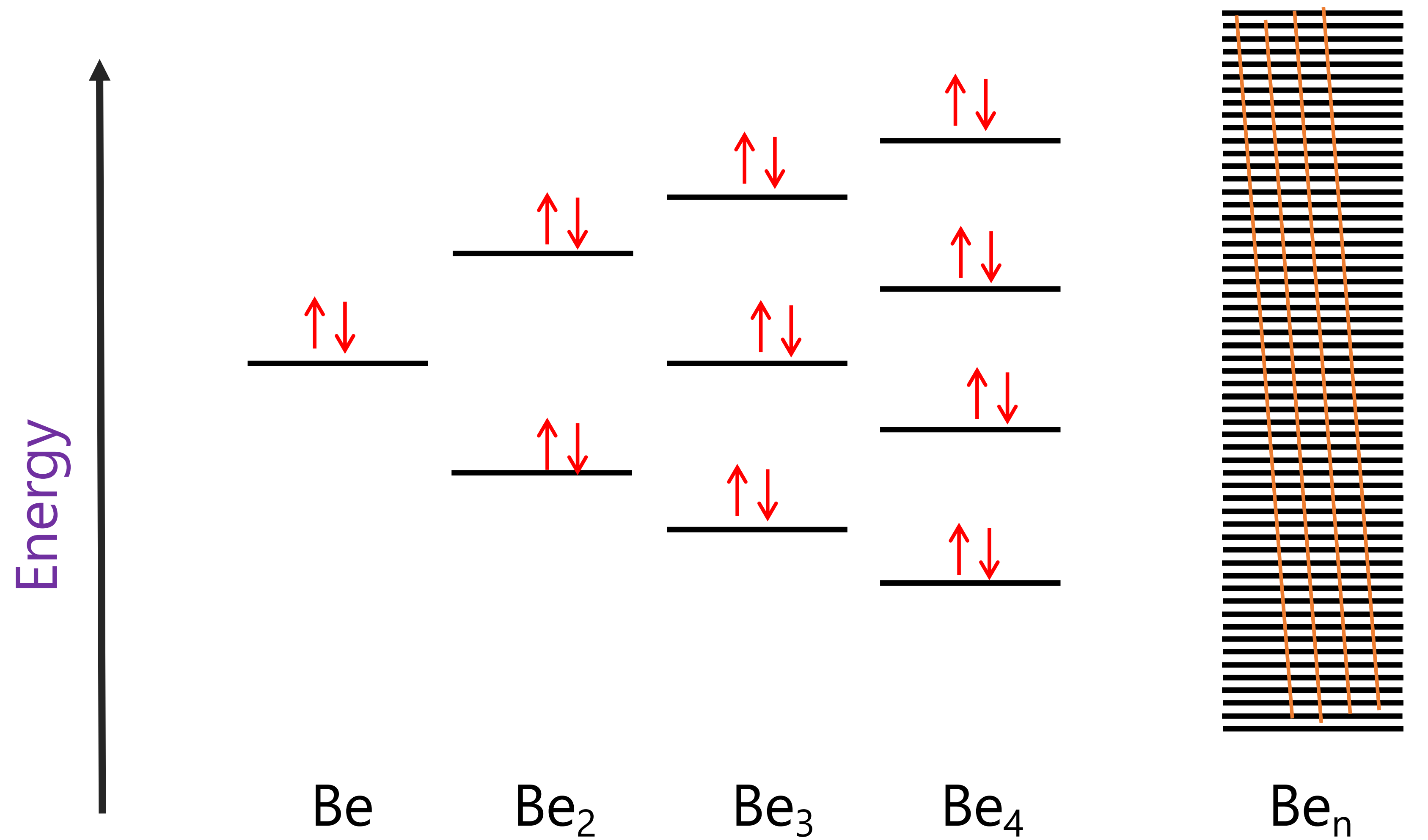


* Small energy gaps enable easy excitation and "mobile" electrons *
(partially filled energy band enables conductivity)

Band Theory Group 2 Metals

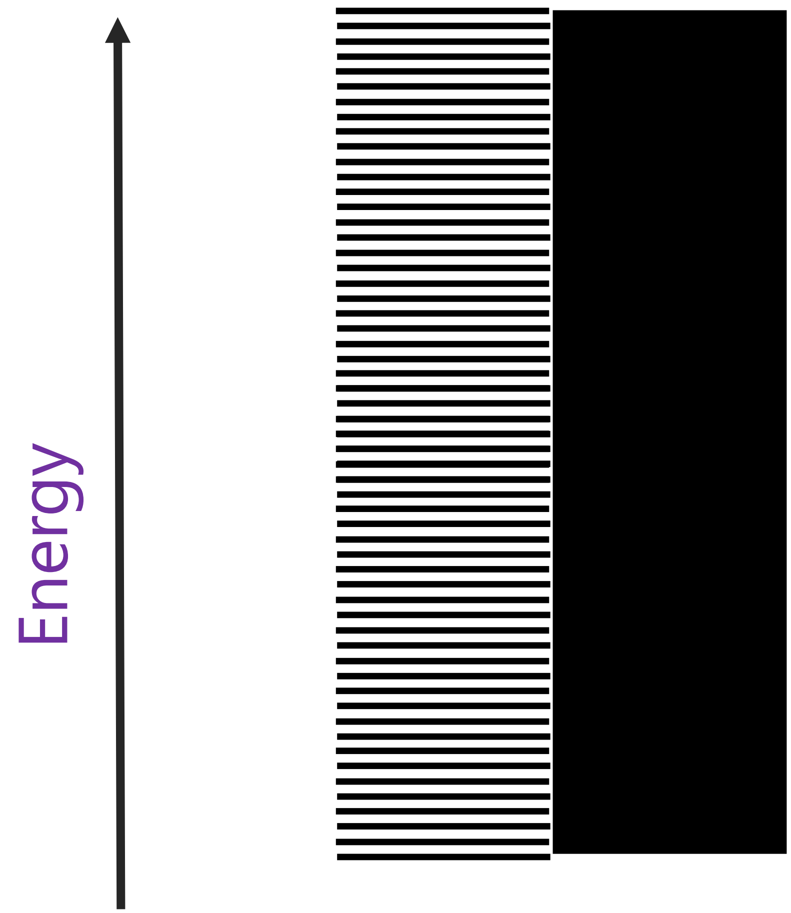
Be $2s^2$

Be_n (metal): ***n*** 2s AOs = ***n*** MOs (***2n*** valence electrons)



Be: Only using 2s Energy Band

Be$_n$ (metal): ***n*** 2s AOs = ***n*** MOs (***2n*** valence electrons)



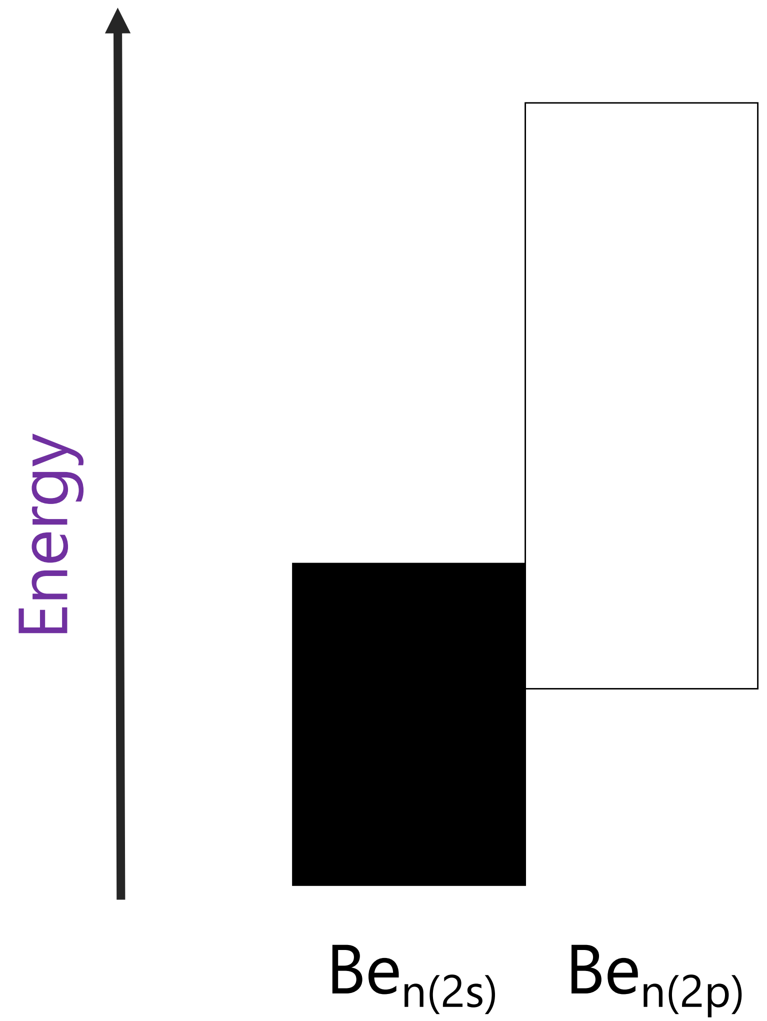
Valence shell of Be
$2s^2\ 2p^0$

Valence Band (2s)
filled MOs

* 2s band completely filled… but 2p band is empty!*

Be with 2s and 2p Energy Bands

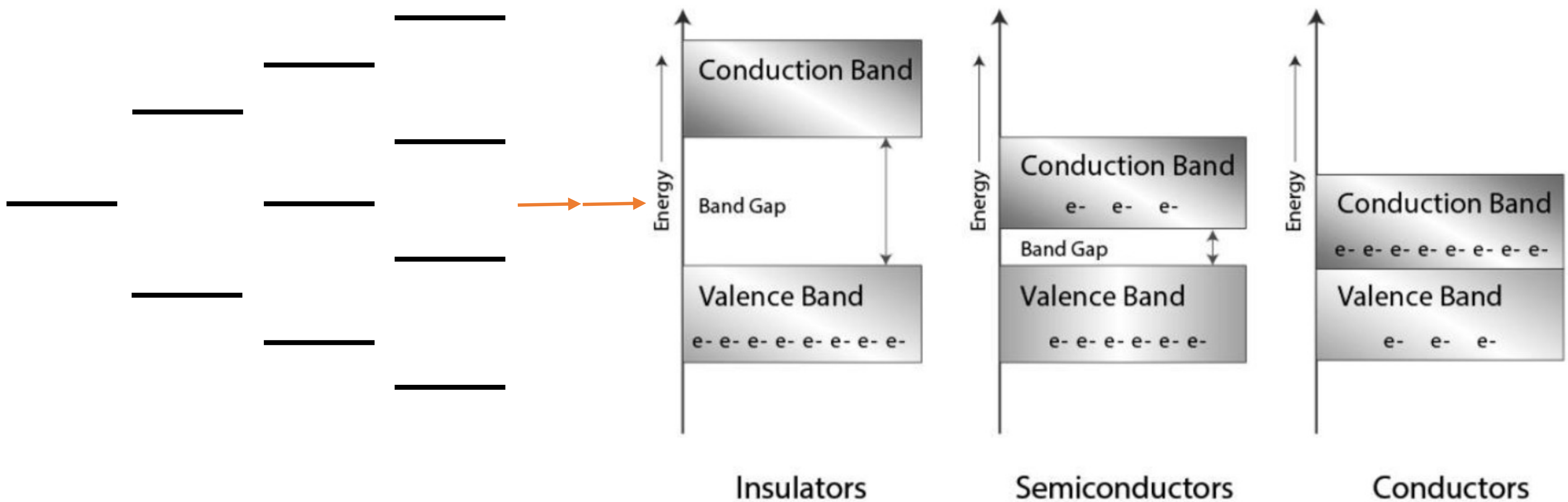
Be_n (metal): ***n*** 2s + ***3n*** 2p AOs = ***4n*** MOs (***2n*** valence electrons)



Conduction Band (2p)
empty MOs

Valence Band (2s)
filled MOs

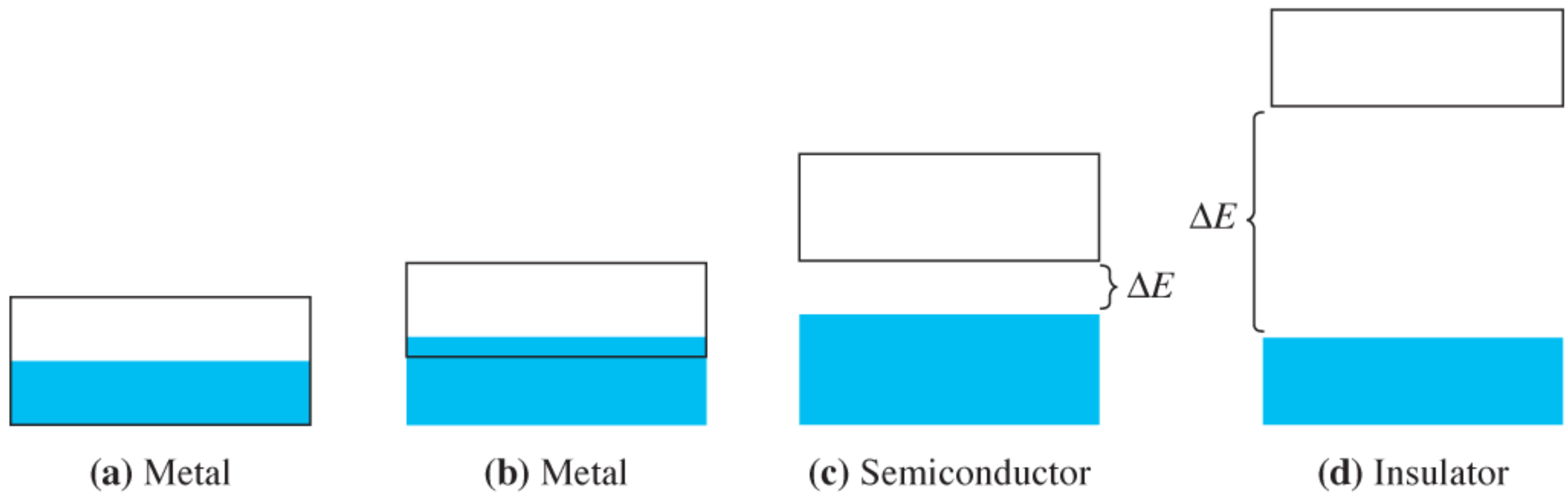
Band Theory: Conductivity



Conductivity

Conductivity depends upon the size of the energy “gap” between valence and conduction band

Metals (conductors) – no band gap, “free” electrons (no covalent bonds)
Semiconductors – small band gap, bonding has more covalent character
Insulators – large band gap, strongly held electrons in covalent bonds



Practice Question 2

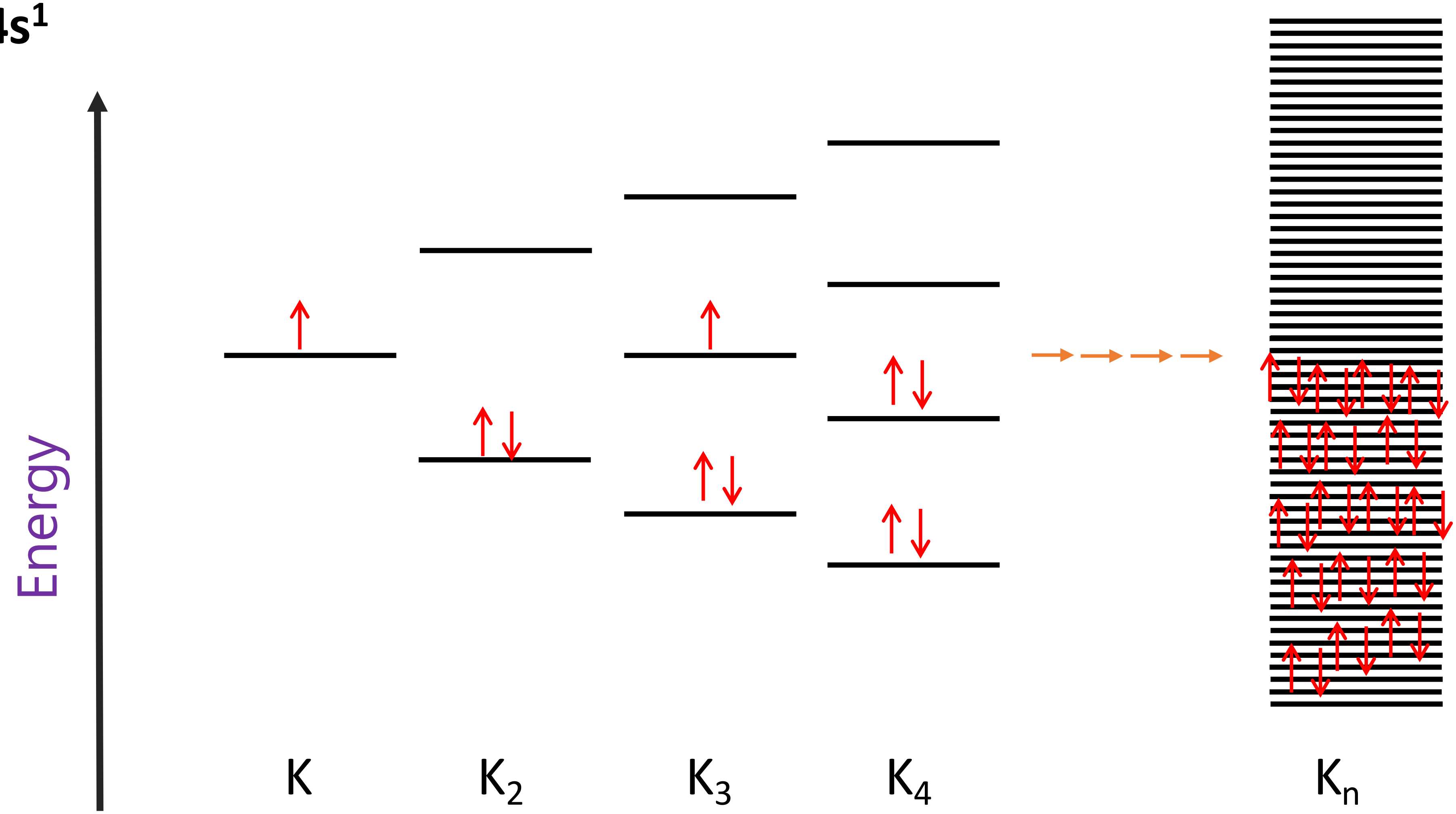
a) Draw the band structure of potassium and silicon.

b) One of these two elements is a semiconductor. Which one? Explain your choice.

Practice Question 2

a) Draw the band structure of potassium and silicon.

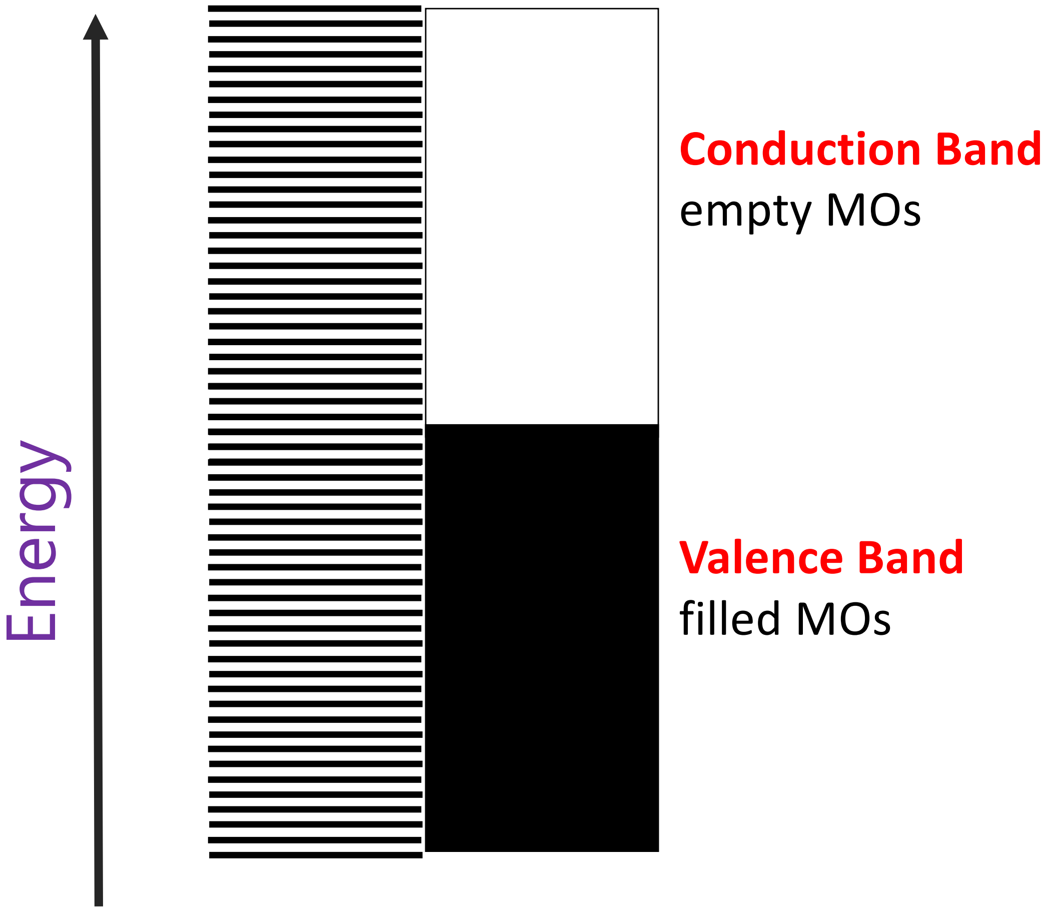
K 4s[1]

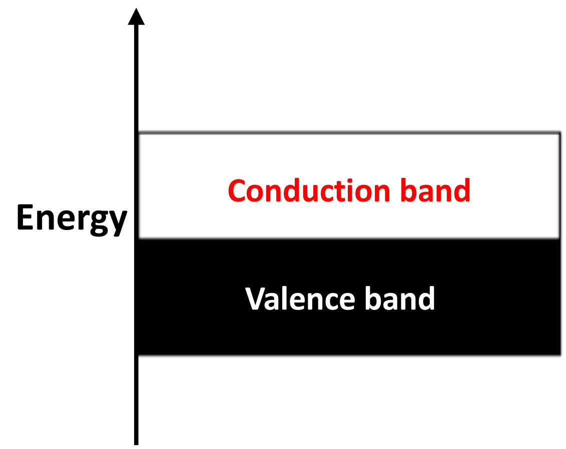


K 4s Energy Band

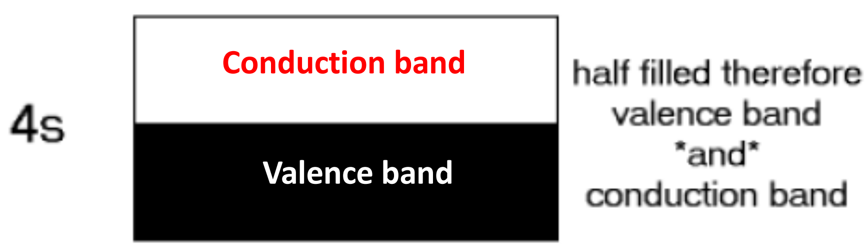
a) Draw the band structure of potassium and silicon.

K $4s^1$ $\quad$ **K_n (metal)**: ***n*** 4s AOs = ***n*** MOs (***n*** valence electrons)





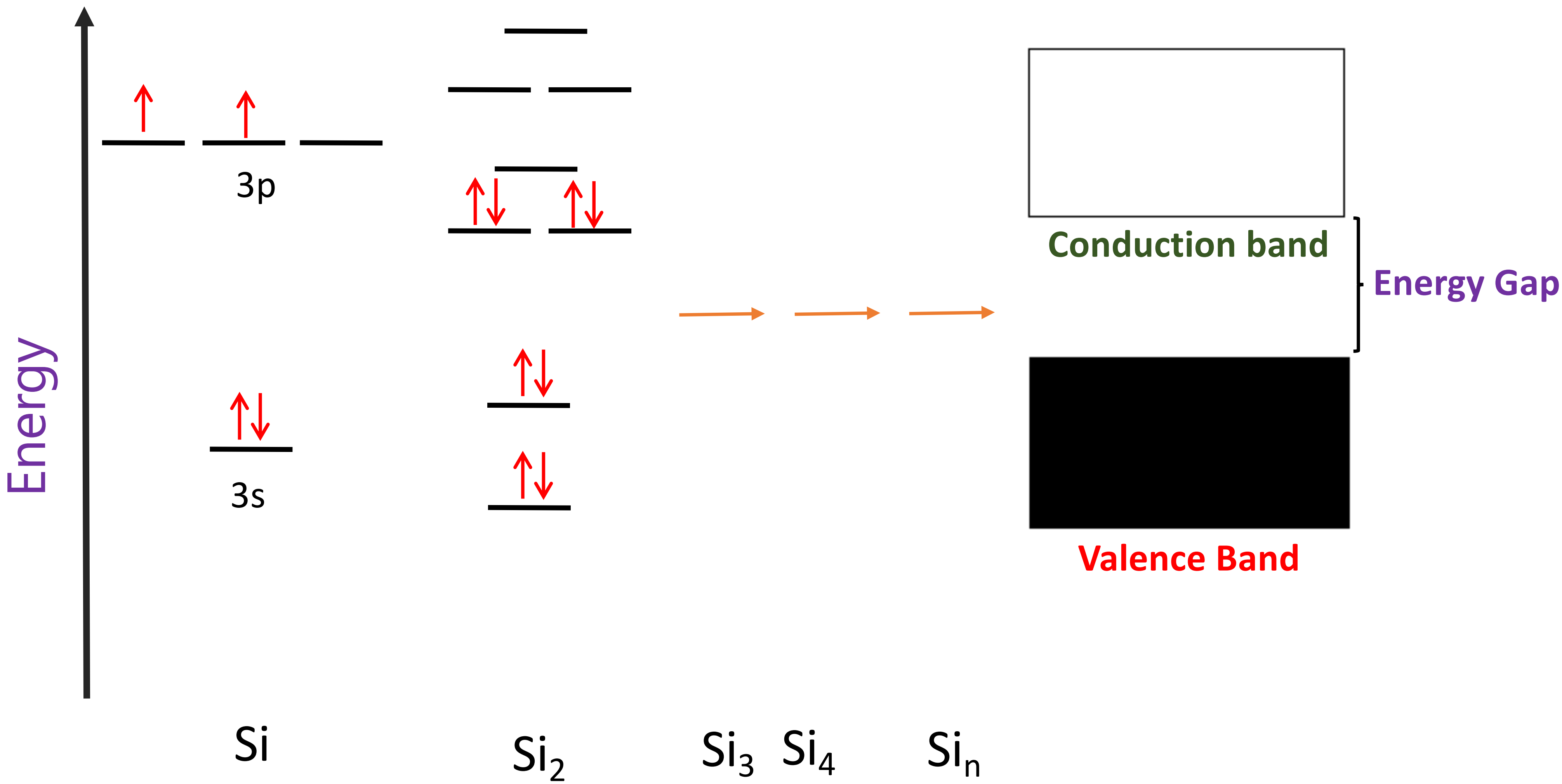
Band structure of K



Practice Question 2

a) Draw the band structure of potassium and silicon.

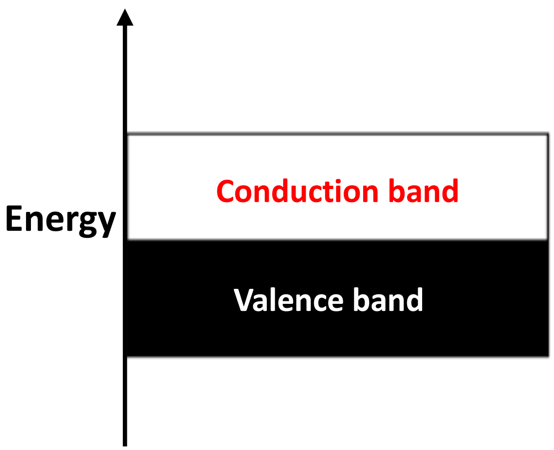
Si $3s^2$ $3p^2$



Practice Question 2

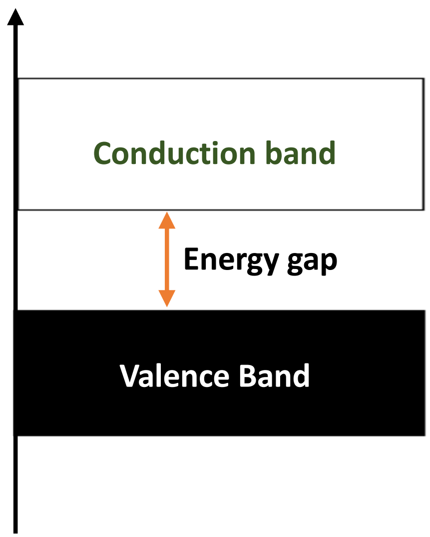
a) Draw the band structure of potassium and silicon.

b) One of these two elements is a semiconductor. Which one? Explain your choice.



Band structure of K

K - Conductor



Band structure of Si

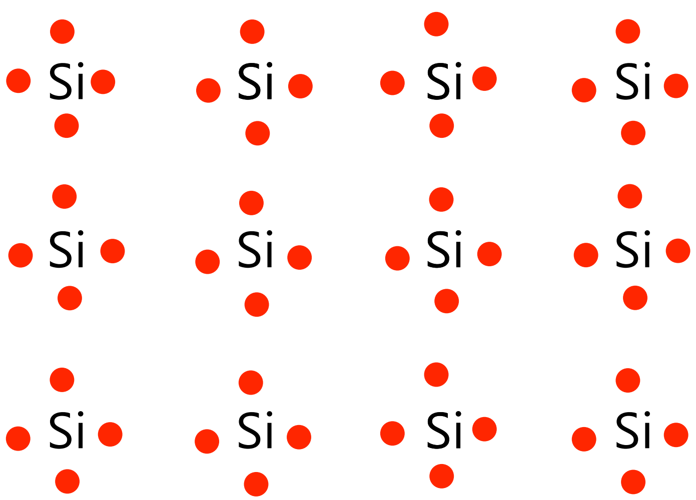
Si - semiconductor

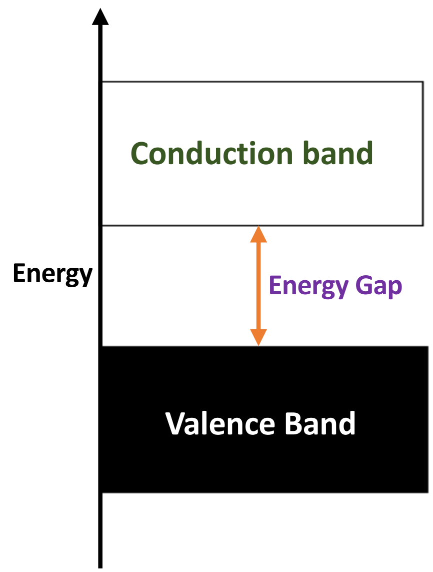
Practice Question 3

Germanium has the same structure as silicon. A small amount of gallium is added to a sample of germanium to improve its ability to conduct electricity.

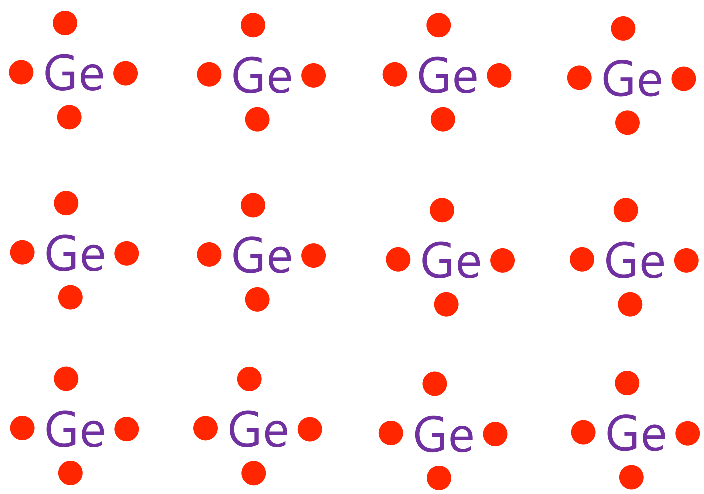
a) Is this an example of a *p*-type semiconductor or an *n*-type semiconductor?
(b) Explain how the addition of gallium increases conductivity.

Si $3s^2$ $3p^2$





Ge $4s^2$ $4p^2$



Practice Question 3

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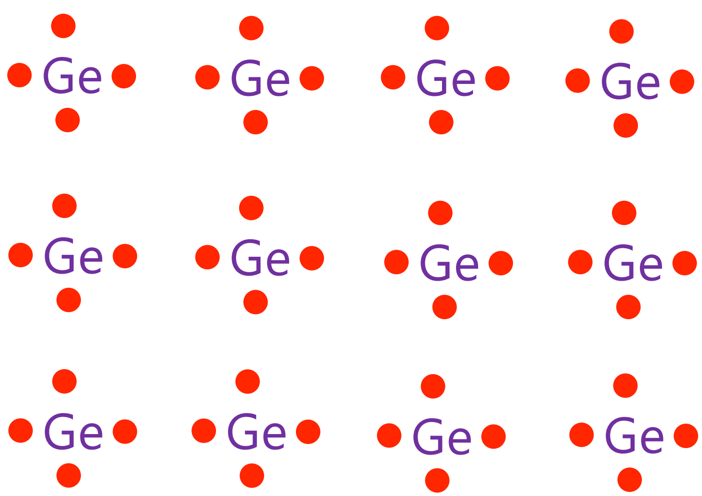
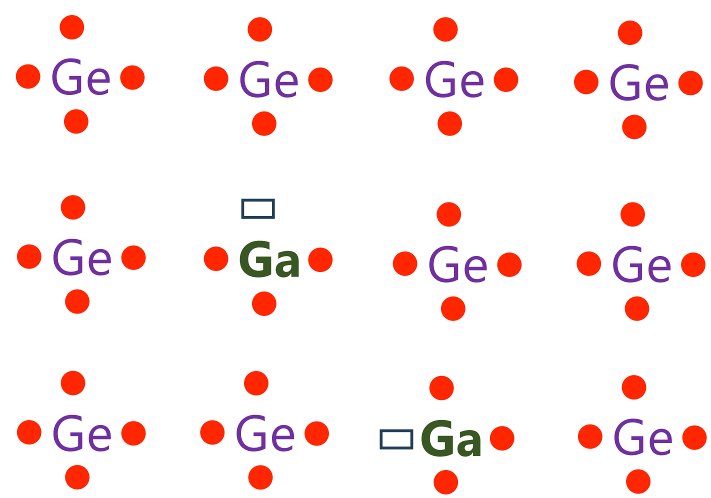
Ge $4s^2$ $4p^2$



Ga $4s^2$ $4p^1$



p-type semiconductor

Practice Question 3

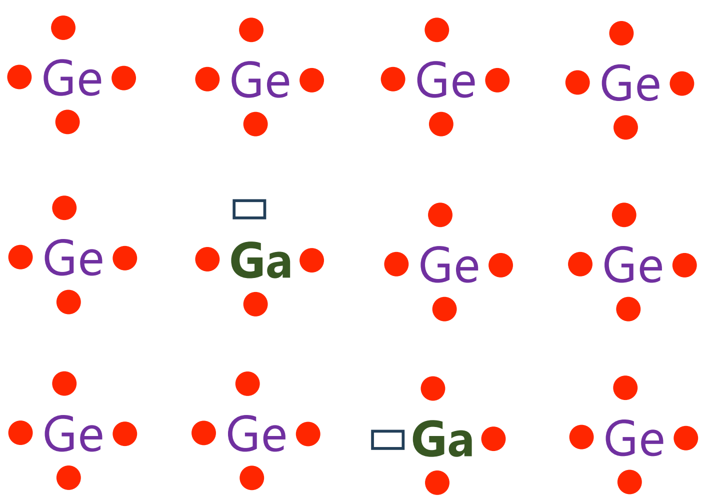
Germanium has the same structure as silicon. A small amount of gallium is added to a sample of germanium to improve its ability to conduct electricity.

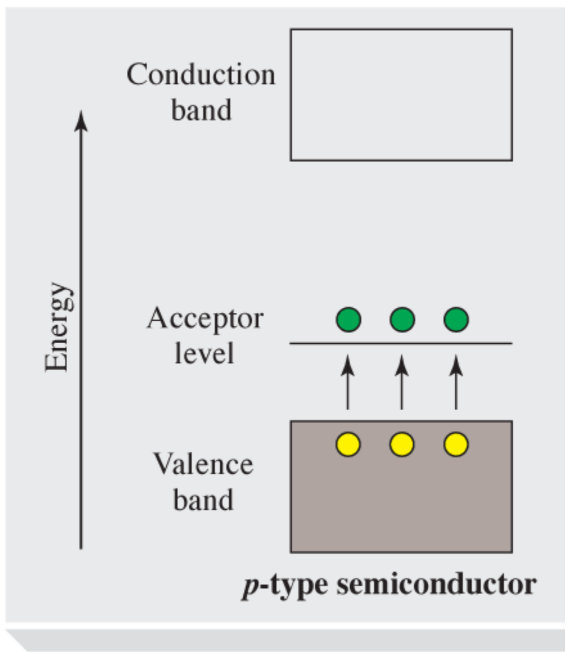
a) Is this an example of a *p*-type semiconductor or an *n*-type semiconductor?

(b) Explain how the addition of gallium increases conductivity.

Ge $4s^2\ 4p^2$

Ga $4s^2\ 4p^1$





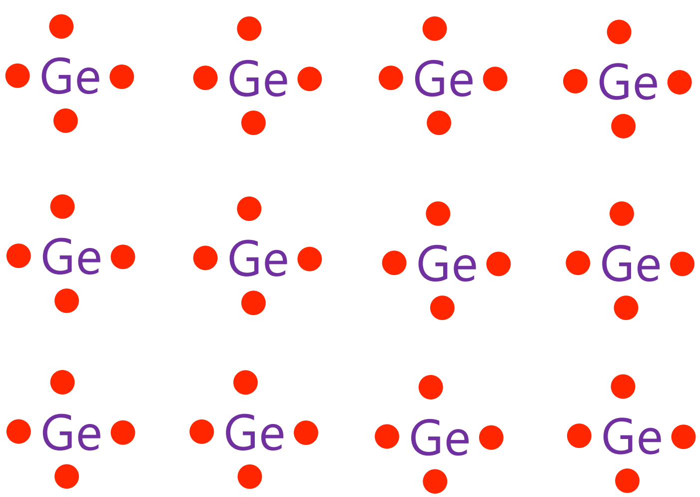
Bonus Practice Question

Identify the following as p-type, n-type or undoped semiconductors:

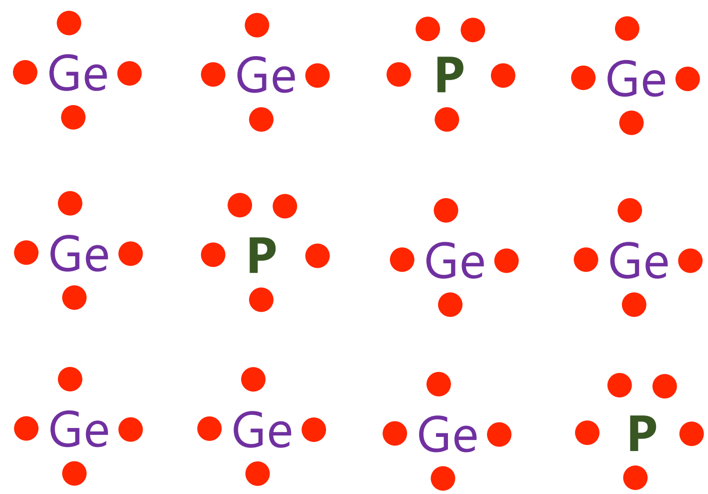
a) Ge doped with P **b) InSb doped with Te** **c) GaP**

a) Ge doped with P

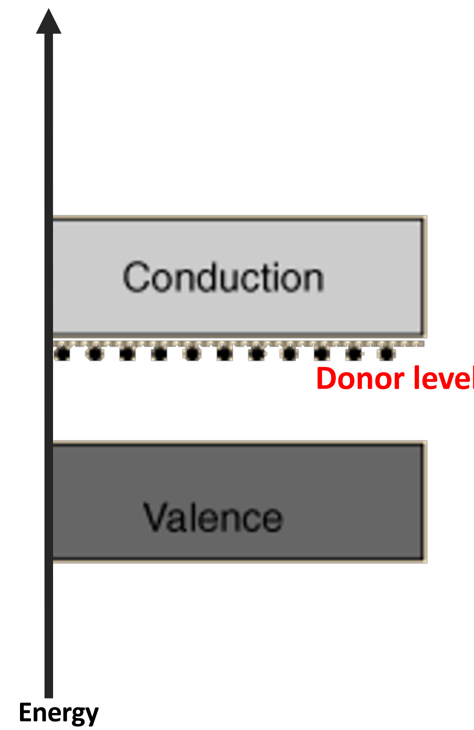
Ge $4s^2\ 4p^2$



P $3s^2\ 3p^3$



n-type semiconductor



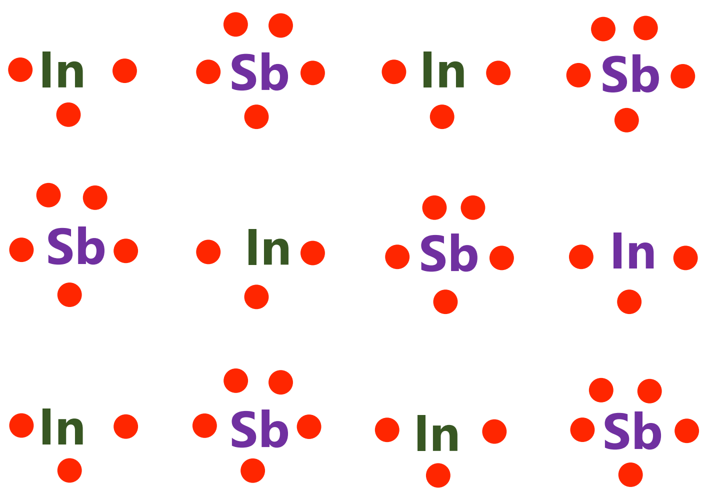
Bonus Practice Question

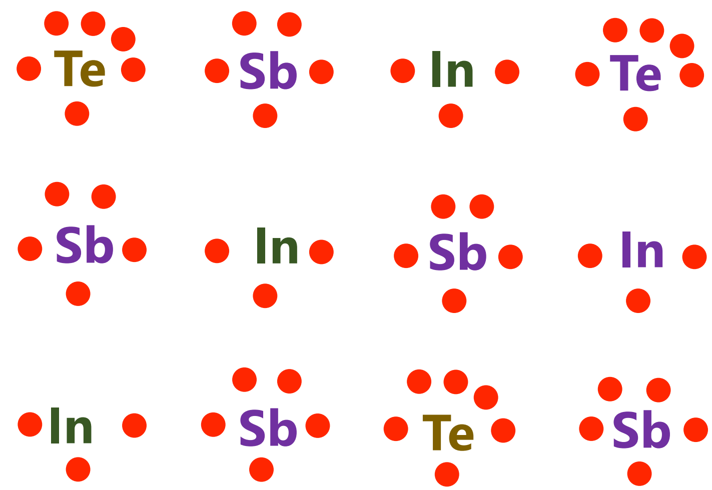
Identify the following as p-type, n-type or undoped semiconductors:

a) Ge doped with P **b) InSb doped with Te** **c) GaP**

b) InSb doped with Te

In $5s^2\ 5p^1$ **Sb $5s^2\ 5p^3$** **Te $5s^2\ 5p^4$**





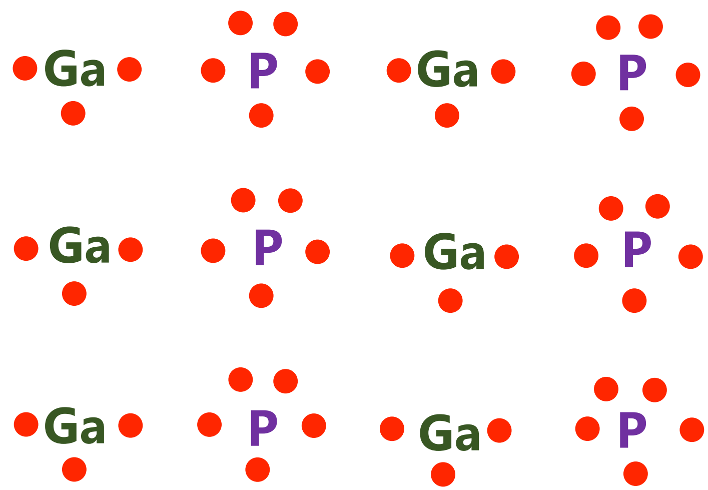
n-type semiconductor

Bonus Practice Question

Identify the following as p-type, n-type or undoped semiconductors:

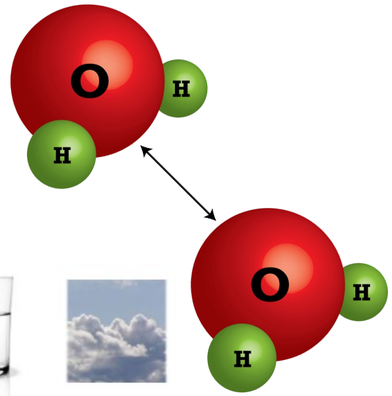
a) Ge doped with P **b) InSb doped with Te** **c) GaP**

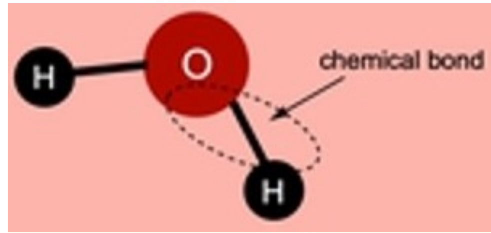
c) GaP **Ga $4s^2$ $4p^1$** **P $3s^2$ $3p^3$**



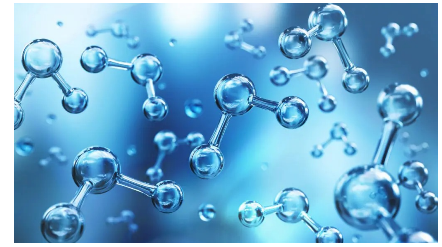
undoped semiconductor

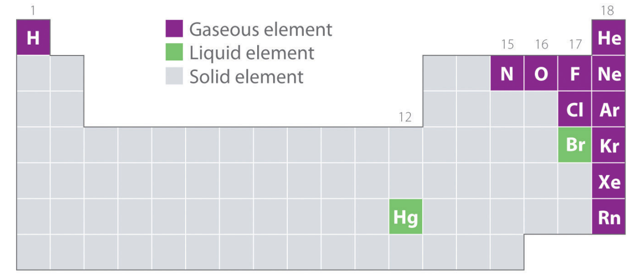
Intermolecular Forces

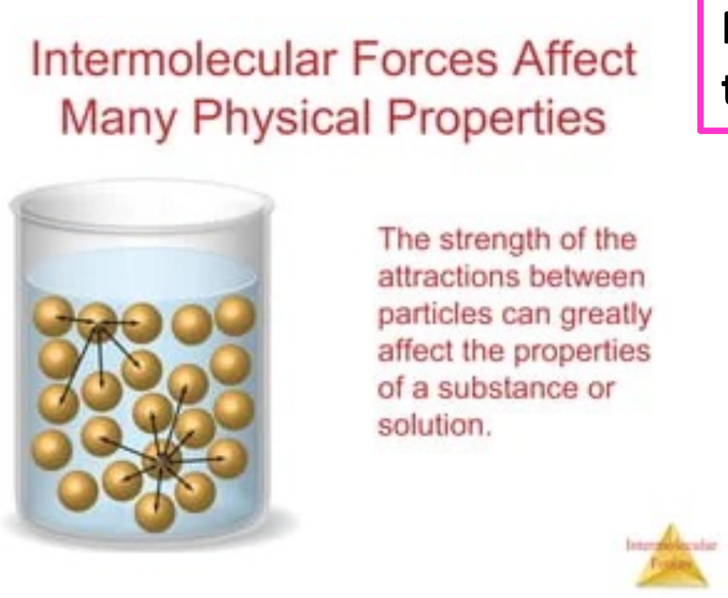




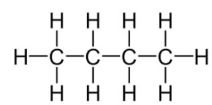
Intramolecular force

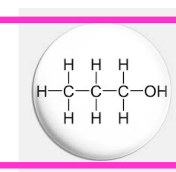




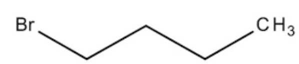


Increased intermolecular forces – Increased boiling point
More interaction between molecules, more heat needed to change from liquid to gaseous state.

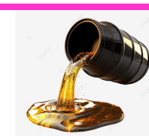




Intermolecular forces affect how soluble a compound will be in a solvent (water, ethanol, etc) – Why does salt dissolve in water?



Intermolecular forces affect viscosity and other physical properties of molecules.



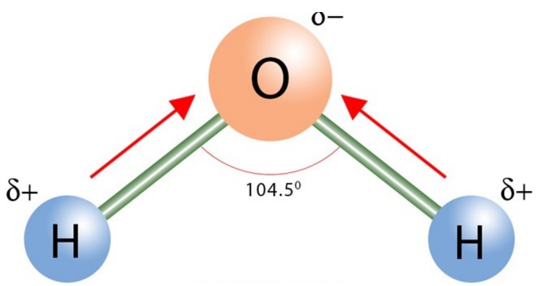
Intermolecular forces <u>between</u> molecules depend upon the interaction <u>between</u> molecules.

These interactions depend upon polarity of a molecule and polarizability.

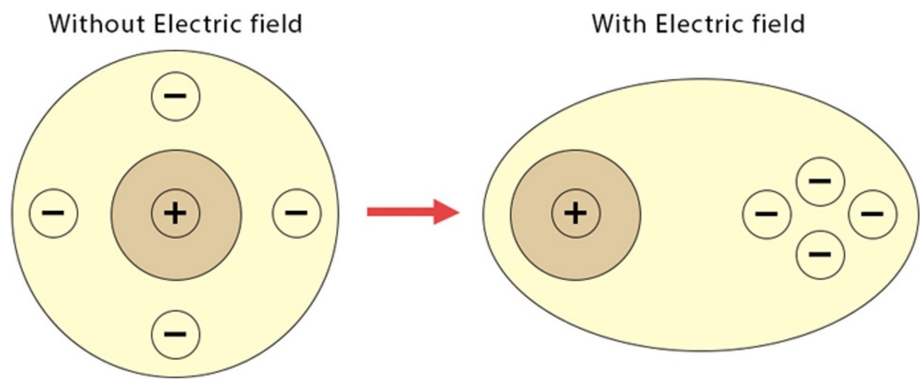
- **Molecules**
  - **Non-polar**
    - Homonuclear diatomic molecules: H_2, O_2, Cl_2 etc; ***and*** Polyatomic molecules with bond polarity cancelled: CO_2, BF_3, CCl_4 etc.
    - Hydrocarbons: alkanes, alkenes, alkynes, benzene and benzene derivatives.
  - **Polar**
    - Heteronuclear diatomic molecules: HF, HBr etc; ***and*** Polyatomic molecules with asymmetric shape: H_2O, SF_4 etc.
    - Organic compounds with functional groups like: R-O-R, C=O, OH, COOH, NH_2 etc.

Intermolecular forces **between** molecules depend upon the interaction **between** molecules.

These interactions depend upon polarity of a molecule and polarizability



Polar Molecule



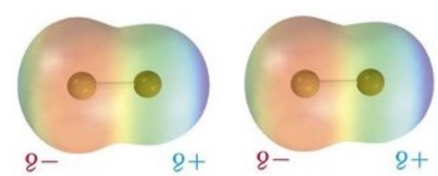
Larger atoms have more loosely held valence electrons are more polarizable than smaller atoms.

Fluorine, for example, has more tightly held electrons than iodine.

F_2 molecules will have smaller attractive force between them, compared to I_2 molecules.

It is easier to create a temporary instantaneous dipole in I_2 than F_2.

Two iodine molecules



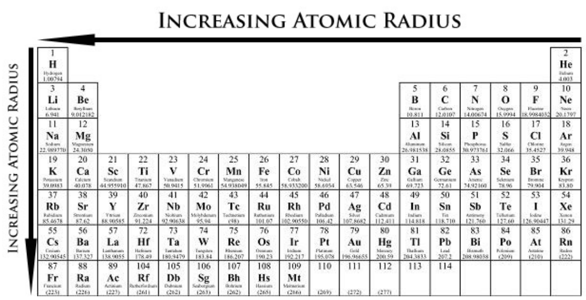
Polarizability is a measure of how the electron cloud in a molecule responds to changes in its electronic environment

Polarizability

How easily can an electron cloud be distorted

Down a group: Polarizability increases

Across a period: Polarizability decreases



Cations: Less polarizable than their atoms

Anions: More polarizable than their atoms

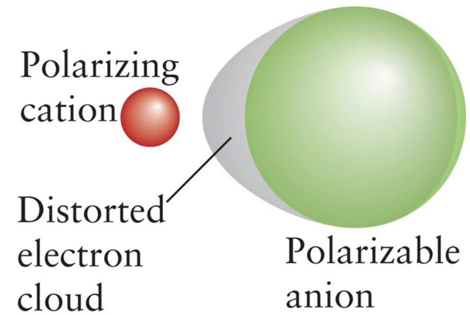
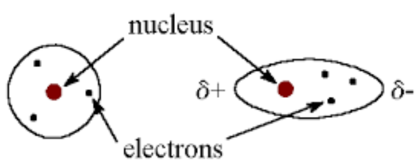


Figure 2D.4
Atkins, *Chemical Principles: The Quest for Insight*, 7e
W. H. Freeman & Company, © 2016 by P. W. Atkins, L. L. Jones, and L. E. Laverman

Intermolecular Forces

Nonbonding (Intermolecular)			kJ/mol	
Ion-dipole		Ion charge–dipole charge	40–600	$Na^{+}\cdots O(H)_2$
H bond	$\overset{\delta-}{—A}—\overset{\delta+}{H}\cdots\cdots\overset{\delta-}{:B}—$	Polar bond to H–dipole charge (high EN of N, O, F)	10–40	$:\ddot{O}(H)—H\cdots:\ddot{O}(H)—H$
Dipole-dipole		Dipole charges	5–25	$I—Cl\cdots I—Cl$
Ion–induced dipole		Ion charge–polarizable e^- cloud	3–15	$Fe^{2+}\cdots O_2$
Dipole–induced dipole		Dipole charge–polarizable e^- cloud	2–10	$H—Cl\cdots Cl—Cl$
Dispersion (London)		Polarizable e^- clouds	0.05–40	$F—F\cdots F—F$



symmetrical distribution

unsymmetrical distribution

Type of Force	Applied to
Dispersion Forces	All molecules
Dipolar Forces	Polar molecules
Hydrogen Bonding	Polar molecules with N – H, O – H or F – H bond

Practice Question 4: Intermolecular Forces

Which intermolecular forces are present in the following compounds?

1. HCl

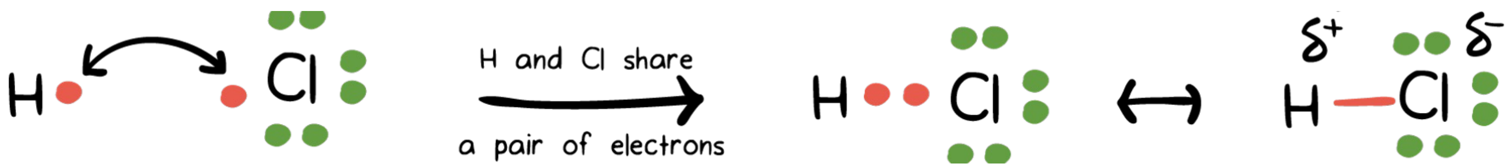
2. Ne

3. HF

Practice Question 4: Intermolecular Forces

Which intermolecular forces are present in the following compounds?

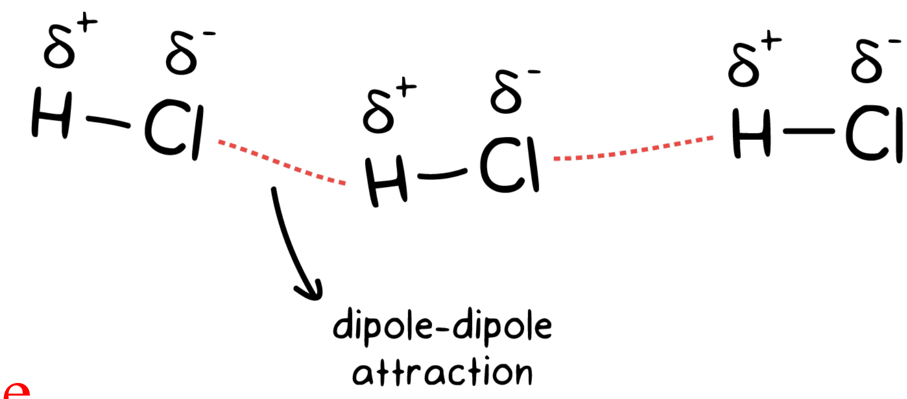
1. HCl **Determine if it is polar. Look at the electronegativity difference.**



Polar Molecule

Dipole – dipole forces

Dispersion forces



HCl is a polar molecule.
It will have dispersion forces and dipole-dipole forces.
No H-bonding since H is bonded to Cl, not to N/O/F

Practice Question 4: Intermolecular Forces

Which intermolecular forces are present in the following compounds?

1. HCl

2. Ne

Determine if it is polar. Look at the electronegativity difference.

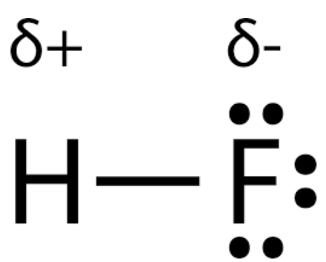
Nonpolar

Dispersion forces

Nonpolar so it will have only dispersion forces.

3. HF

Determine if it is polar. Look at the electronegativity difference.

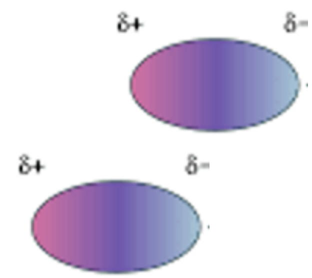


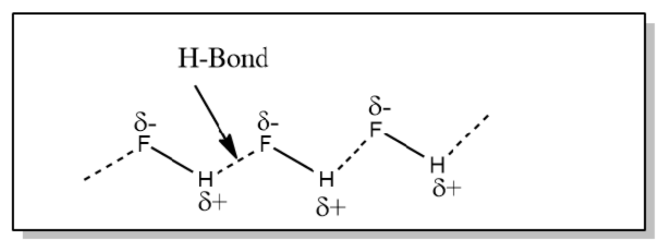
Polar Molecule

Dispersion forces

Dipole – dipole forces

Hydrogen bonding





Practice Question 4: Intermolecular Forces

Which intermolecular forces are present in the following compounds?

1. HCl

Dispersion forces and Dipole-dipole forces.

2. Ne

Dispersion forces

3. HF

Dispersion forces, Dipole-dipole forces, Hydrogen bonding

Practice Question 5

Which of these molecules will have Hydrogen bonding?

$CH_3CH_2CH_2OH$

CH_3CHO

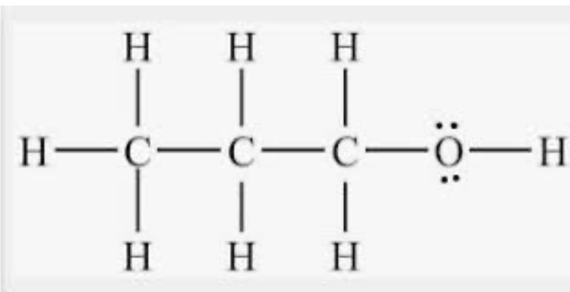
CH_3CH_2F

$CH_3CH_2NH_2$

Practice Question 5

Which of these molecules will have Hydrogen bonding?

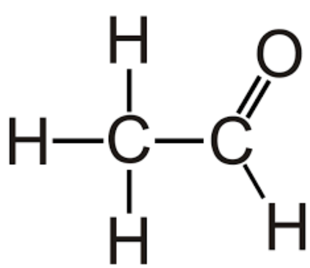
$CH_3CH_2CH_2OH$



Hydrogen bonded to a small highly electronegative element (O)

YES, this molecule will have hydrogen bonding

CH_3CHO



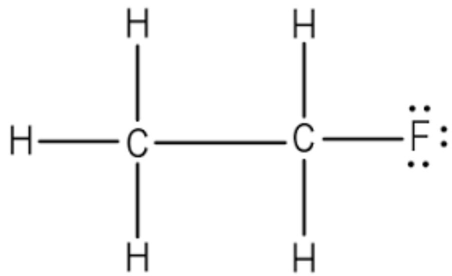
Hydrogen bonded to carbon,
and NOT to a small highly electronegative element

NO, this molecule will NOT have hydrogen bonding

Practice Question 5

Which of these molecules will have Hydrogen bonding?

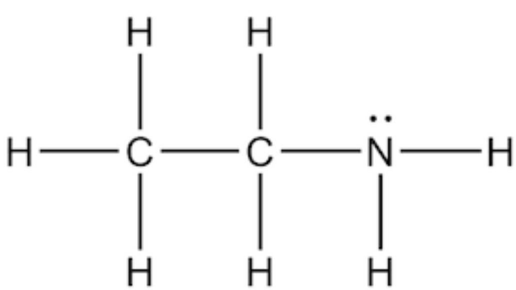
CH_3CH_2F



Hydrogen bonded to carbon,
and NOT to a small highly electronegative element.

NO, this molecule will NOT have hydrogen bonding

$CH_3CH_2NH_2$



Hydrogen bonded to a small highly electronegative element (N)

YES, this molecule will have hydrogen bonding

Practice Question 5

Which of these molecules will have Hydrogen bonding?

$CH_3CH_2CH_2OH$

YES

CH_3CHO

NO

CH_3CH_2F

NO

$CH_3CH_2NH_2$

YES

Practice Question 6

Arrange the following in increasing order of their boiling points?

$CH_3CH_2CH_2CH_2CH_3$ $CH_3C(CH_3)_2CH_3$ $CH_3C(CH_3)_2CH_2OH$

Arrange the following in increasing order of their intermolecular forces?

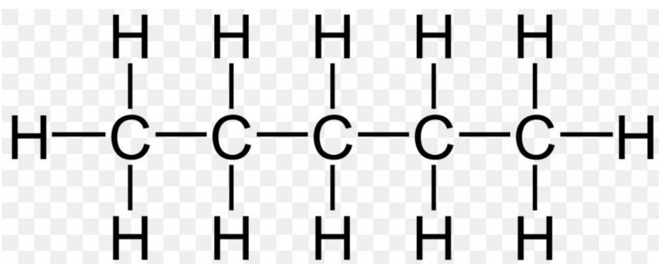
I_2 Br_2 HCl

Practice Question 6

Arrange the following in increasing order of their boiling points?

$CH_3CH_2CH_2CH_2CH_3$ $CH_3C(CH_3)_2CH_3$ $CH_3C(CH_3)_2CH_2OH$

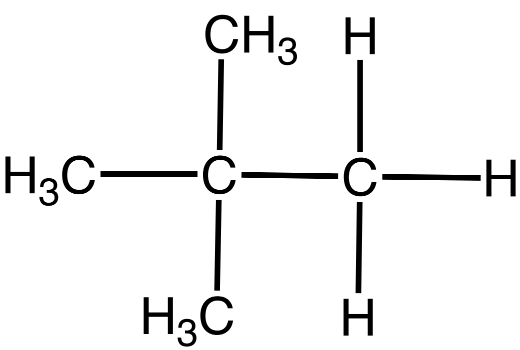
Formula: C_5H_{12}



Nonpolar, Linear molecule, High surface area

Dispersion forces only.

$CH_3C(CH_3)_2CH_3$



Nonpolar, Branched molecule, Low surface area

Dispersion forces only.

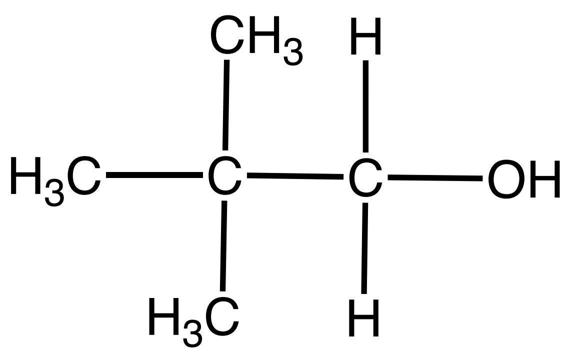
Practice Question 6

Arrange the following in increasing order of their boiling points?

$CH_3CH_2CH_2CH_2CH_3$ $CH_3C(CH_3)_2CH_3$ $CH_3C(CH_3)_2CH_2OH$

Formula: $C_5H_{12}O$

$CH_3C(CH_3)_2CH_2OH$



Polar molecule

Dispersion, Dipole-dipole, Hydrogen bonding

Practice Question 6

Arrange the following in increasing order of their boiling points?

$CH_3CH_2CH_2CH_2CH_3$

Nonpolar, Linear molecule, High surface area

Dispersion forces only.

$CH_3C(CH_3)_2CH_3$

Nonpolar, Branched molecule, Low surface area

Dispersion forces only.

Weakest intermolecular forces

$CH_3C(CH_3)_2CH_2OH$

Polar molecule

Dispersion, Dipole-dipole, Hydrogen bonding

Strongest intermolecular forces

$$CH_3C(CH_3)_2CH_3 < CH_3CH_2CH_2CH_2CH_3 < CH_3C(CH_3)_2CH_2OH$$

Practice Question 6

Arrange the following in increasing order of their boiling points?

$CH_3CH_2CH_2CH_2CH_3$ $CH_3C(CH_3)_2CH_3$ $CH_3C(CH_3)_2CH_2OH$

Arrange the following in increasing order of their intermolecular forces?

I_2 Br_2 HCl

I_2	Br_2	HCl
Nonpolar molecule	**Nonpolar molecule**	**Polar molecule**
Molar mass = (127 x 2) = 254	**Molar mass = (80 x 2) = 160**	
Dispersion forces only	**Dispersion forces only**	**Dispersion forces** **Dipole - dipole forces**

$$Br_2 < I_2 < HCl$$

Revision: Chemical Bonding and Intermolecular Forces

Practice Question

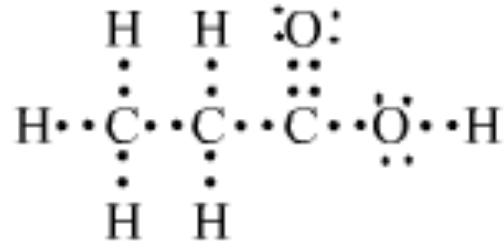
1. Draw the Lewis structure for CH_3CH_2COOH
2. Predict the VSEPR geometry at each of the carbons.
3. Determine a hybridization scheme to rationalize the geometry.
4. Identify the orbitals involved in each bond.

Practice Question

1. Draw the Lewis structure for CH_3CH_2COOH.

CH_3CH_2COOH

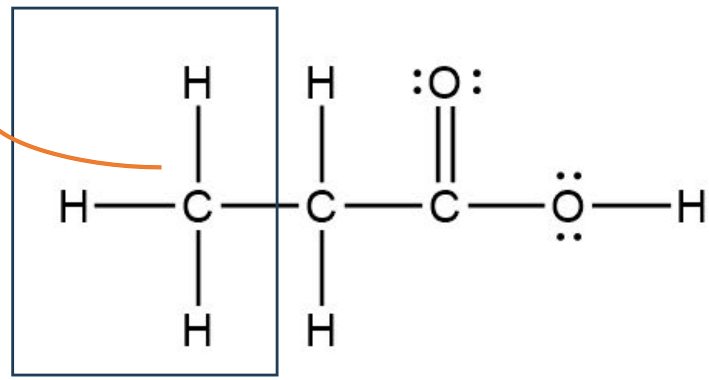
C $2s^2\ 2p^2$
O $2s^2\ 2p^4$
H $1s^1$



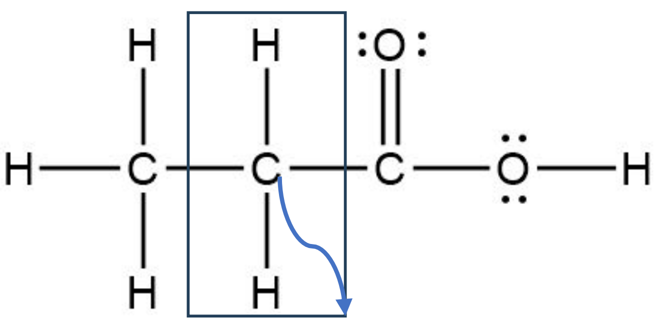
1. Draw the Lewis structure for CH_3CCH.
2. Predict the VSEPR geometry at each of the carbons.

Bond pairs = 4

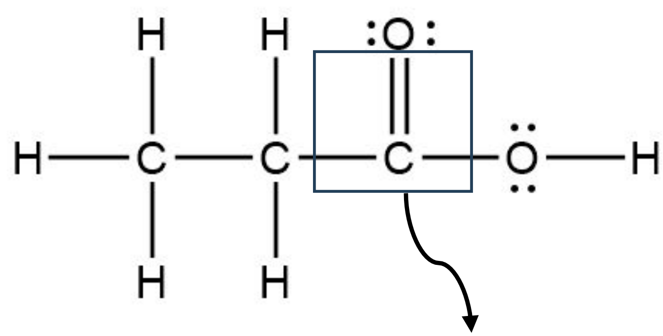
Geometry = Tetrahedral



VSEPR geometry requires the count of bond pairs



Bond pairs = 4
Geometry = Tetrahedral



Bond pairs = 3
Geometry = Trigonal planar

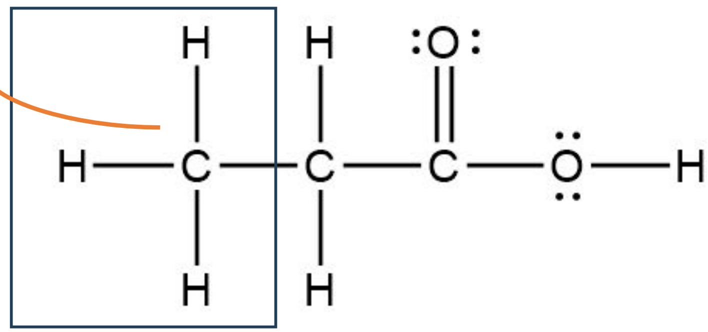
Practice Question

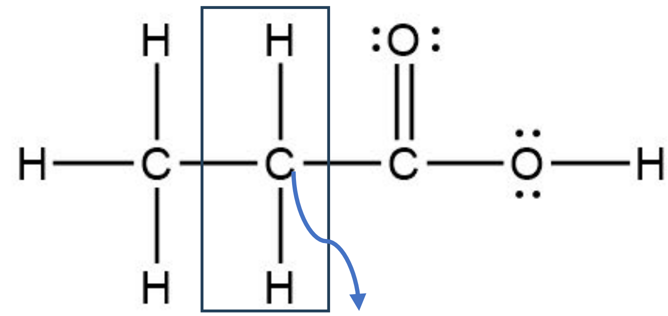
1. Draw the Lewis structure for CH_3CH_2COOH
2. Predict the VSEPR geometry at each of the carbons.
3. Determine a hybridization scheme to rationalize the geometry.
4. Identify the orbitals involved in each bond.

C $2s^2\ 2p^2$
O $2s^2\ 2p^4$
H $1s^1$

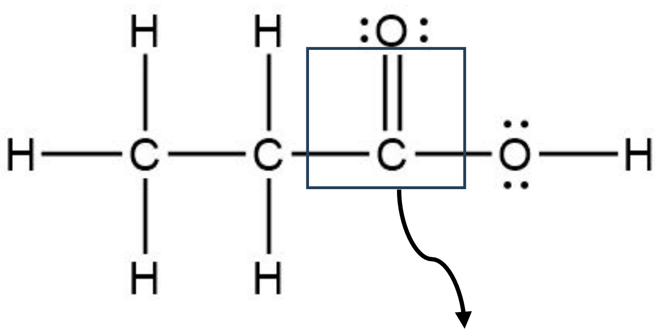
CH_3CH_2COOH

Electron pairs = 4
Hybrid orbitals = 4
Hybridization = sp^3

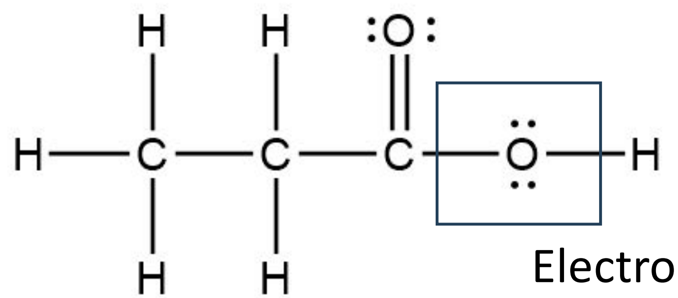




Electron pairs = 4
Hybrid orbitals = 4
Hybridization = sp^3



Electron pairs = 3
Hybridization = sp^2



Electron pairs = 4
Hybridization = sp^3

Practice Question

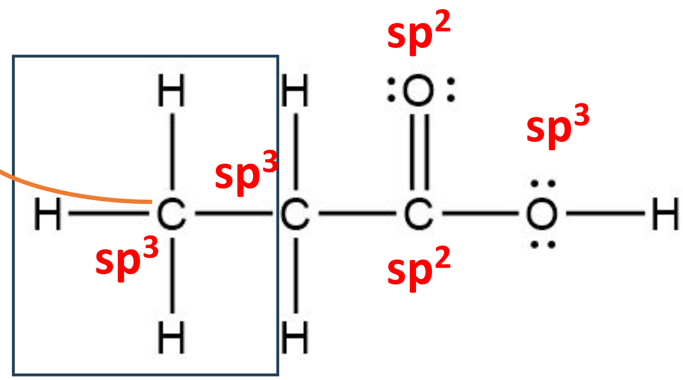
1. Draw the Lewis structure for CH_3CH_2COOH
2. Predict the VSEPR geometry at each of the carbons.
3. Determine a hybridization scheme to rationalize the geometry.
4. Identify the orbitals involved in each bond.

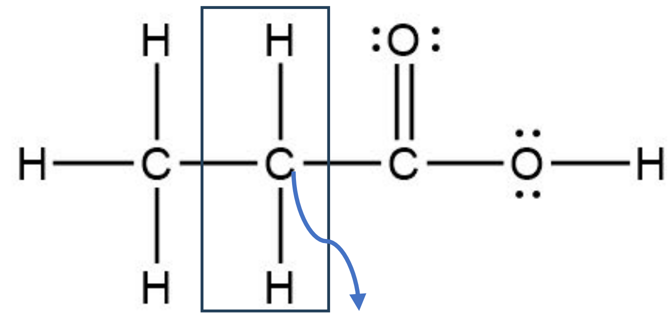
C $2s^2\ 2p^2$
O $2s^2\ 2p^4$
H $1s^1$

CH_3CH_2COOH

Three sp^3-s σ bonds

One sp^3-sp^3 σ bond

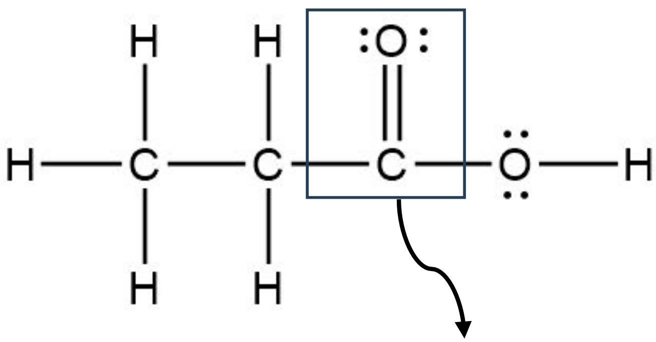




Two sp^3-s σ bonds

One sp^3-sp^3 σ bond

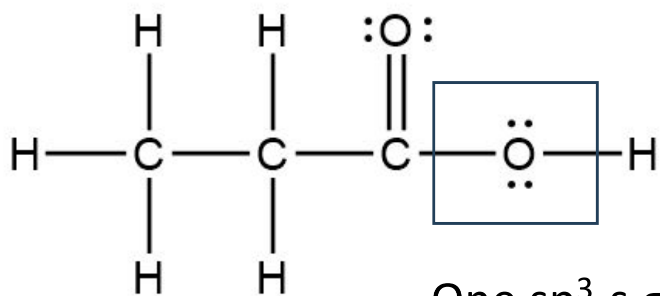
One sp^3-sp^2 σ bond



Two sp^2-sp^3 σ bonds

One sp^2-sp^2 σ bond

One p-p π bond



One sp^3-s σ bond

One sp^3-sp^2 σ bond

Practice Question

Draw MO diagram for CN^-. What is the bond order? Write down its MO electronic configuration and indicate if the molecule will be dia- or paramagnetic.

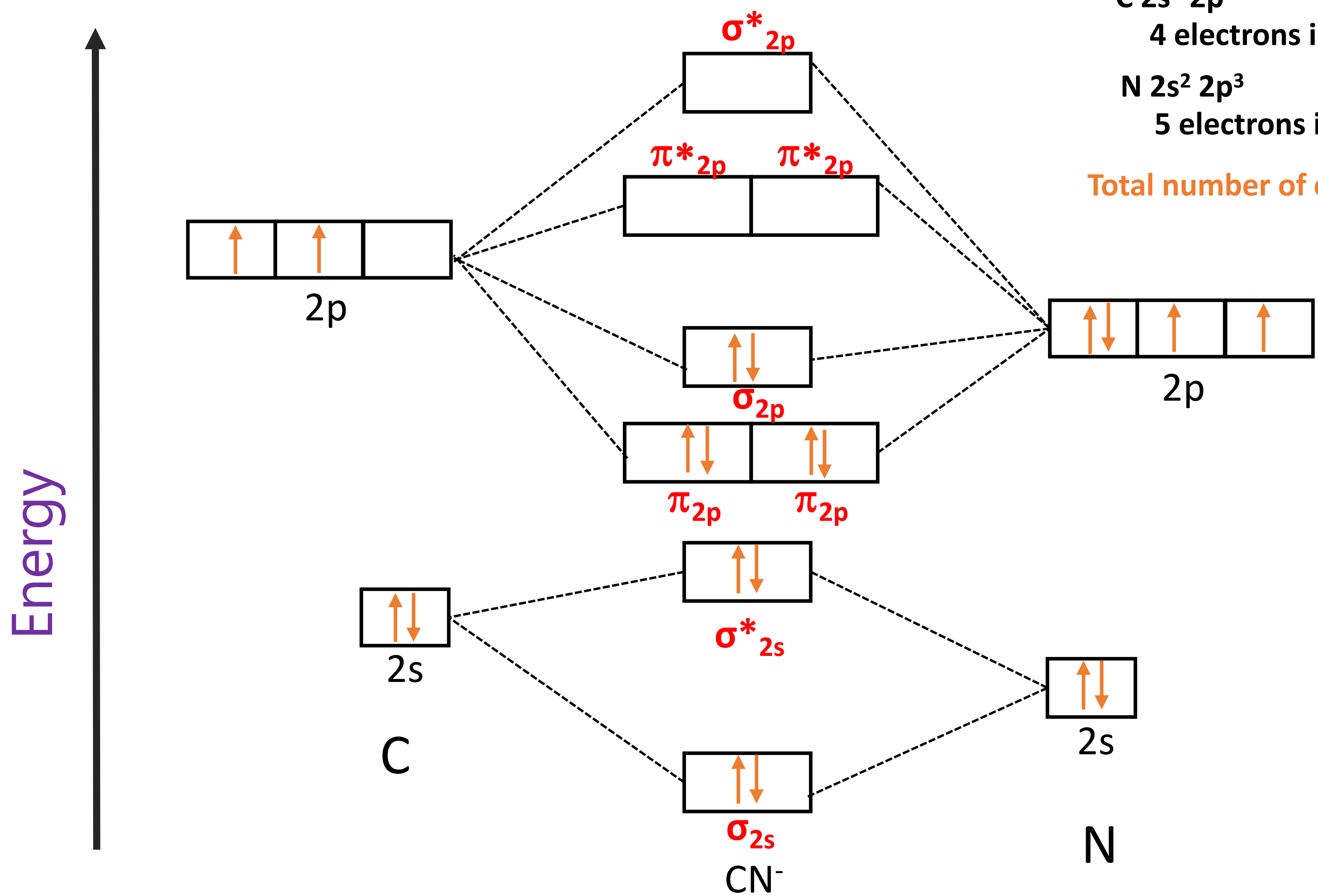
C $2s^2\ 2p^2$

4 electrons in the valence shell

N $2s^2\ 2p^3$

5 electrons in the valence shell

Total number of electrons in CN^- = 10

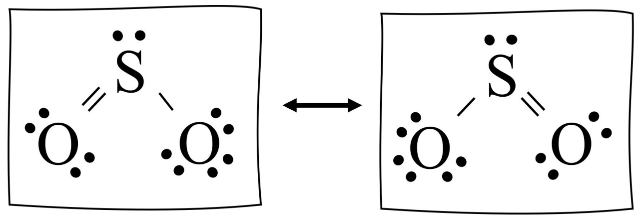


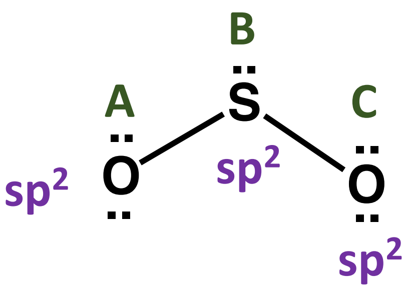
Bond Order = ½ (no. of electrons in bonding orbitals – no. of electrons in antibonding orbitals)

$(\sigma 2s)^2\ (\sigma^* 2s)^2\ (\pi 2p)^4\ (\sigma 2p)^2$ **Bond order in CO = (8–2)/2 = 3** **Diamagnetic**

Resonance

SO_2



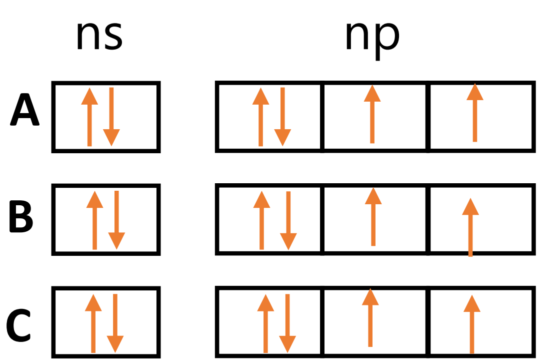


S $3s^2\ 3p^4$

O $2s^2\ 2p^4$

(valence orbitals)

Determine hybridization at each atom center



Number of electron groups = 3 = number of hybrid orbitals = 3 = sp^2

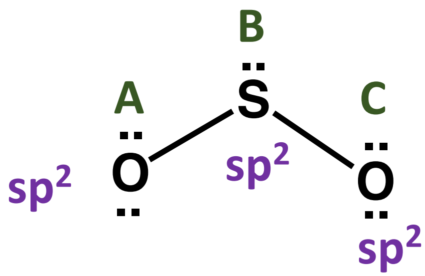
Number of electron groups = 3 = number of hybrid orbitals = 3 = sp^2

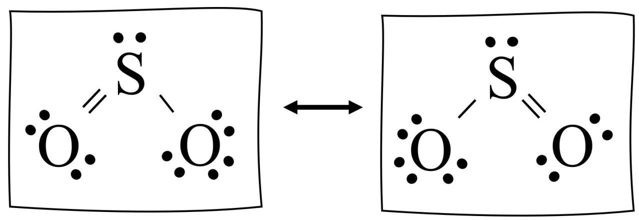
Number of electron groups = 3 = number of hybrid orbitals = 3 = sp^2

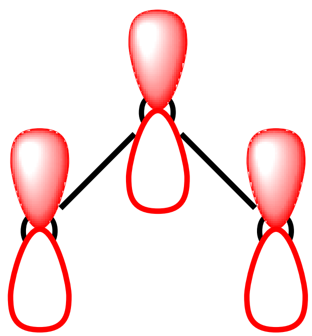
For all the sigma bonds we use valence bond theory and hybridization

- the central Sulfur is sp^2 hybridized
- Two sp^2 – sp^2 sigma bonds with two terminal oxygen atoms
- Third sp^2 orbital contains the lone pair of electrons on sulfur

SO_2 : delocalized π electrons







From LCAO of 3 p orbitals

π* MO

π non-bonding MO

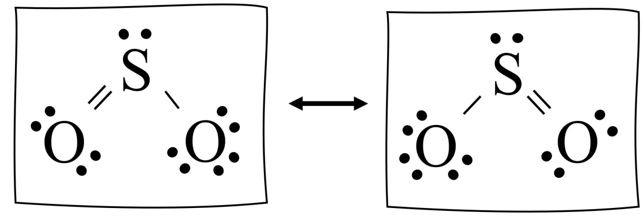
π MO

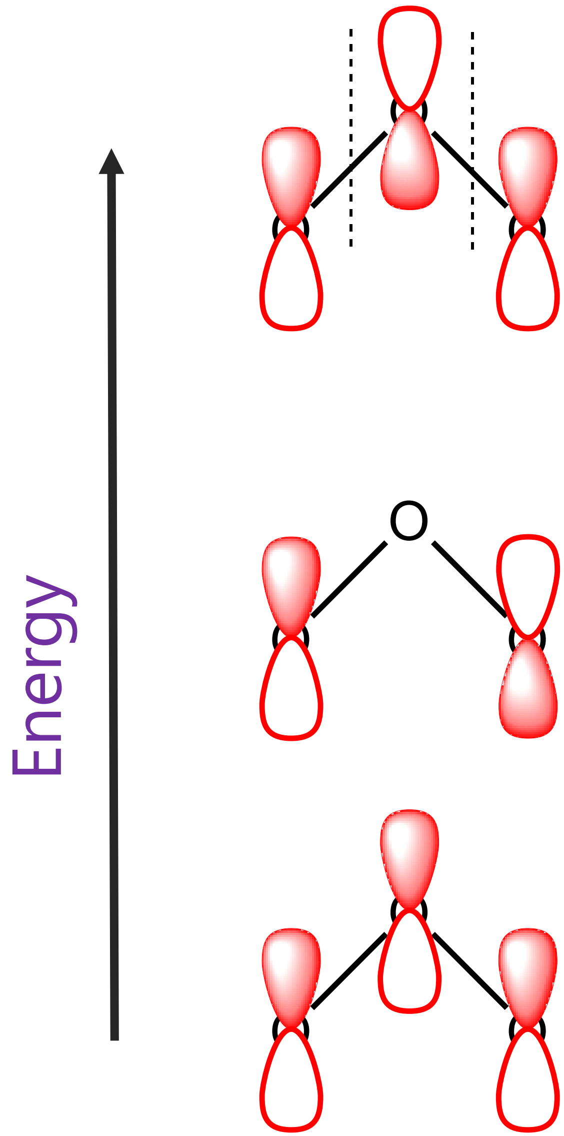
3 π MOs

SO_2 : delocalized π electrons

For hybridization, we removed moving bond (one that was making a double bond on either side) and a moving lone pair of electrons.

These four electrons are delocalized in the structure.

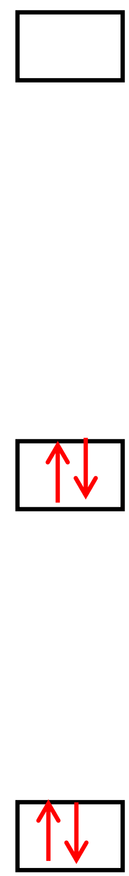




π* MO

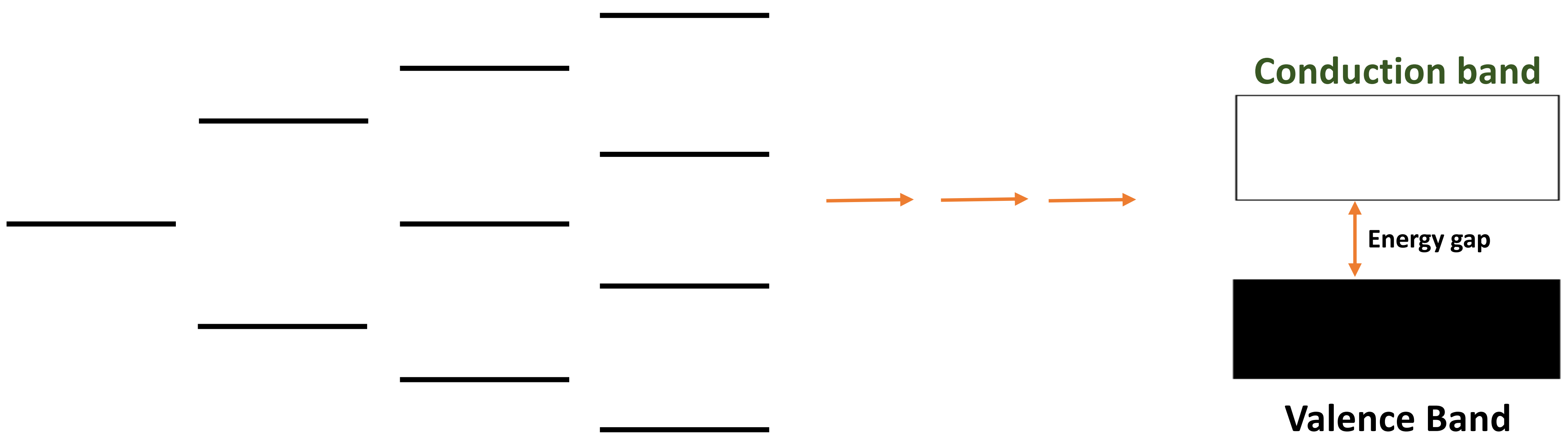
π non-bonding MO

π MO



Graphic displays involve the use of semiconductors which absorb different amounts of energy depending on particle size. This energy is then re-emitted as photons of light. Different particle sizes give different colours.

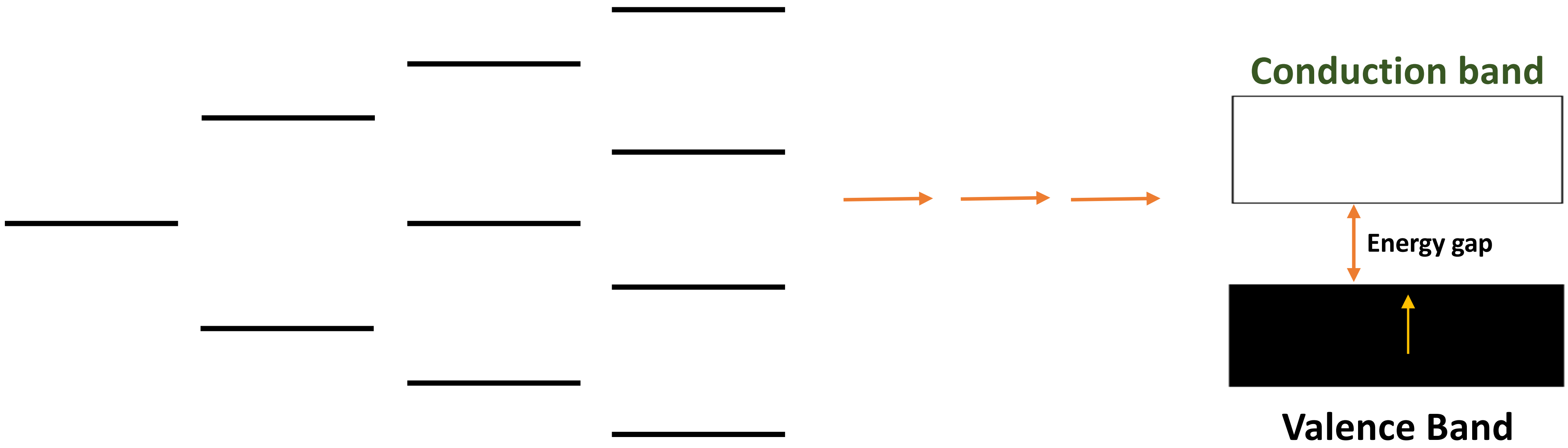
Use band theory to explain why the larger particles produce colours toward the red end of the visible spectrum while smaller particles produce colours toward the violet end.

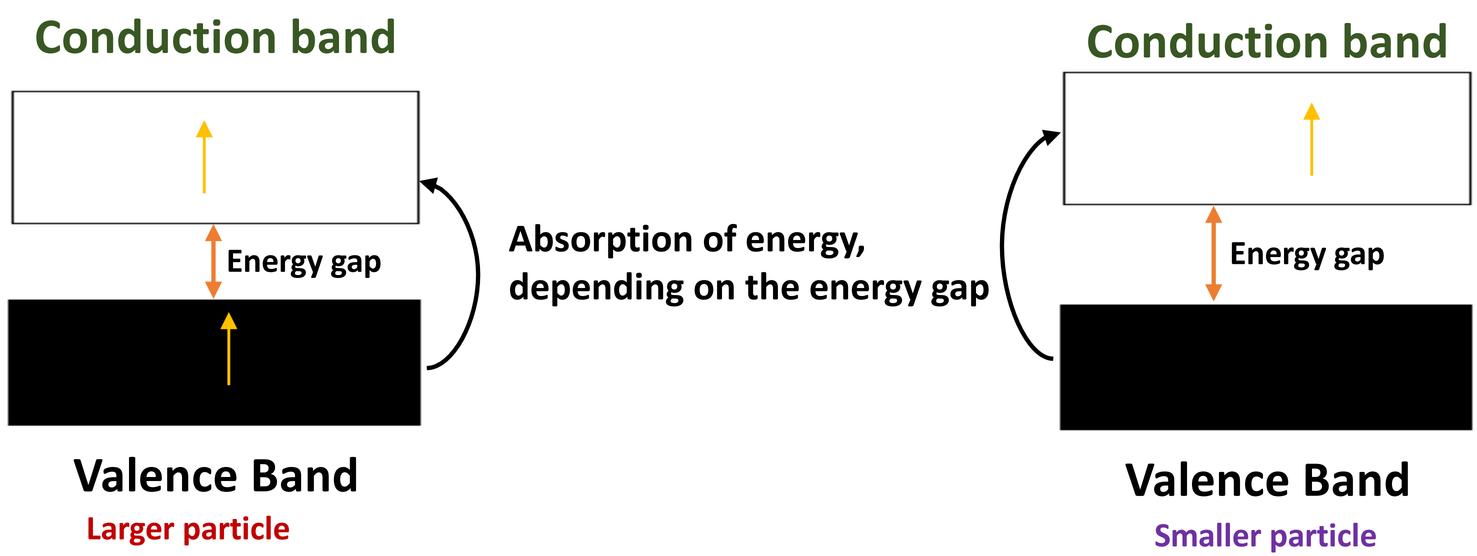


Formation of a Band

Graphic displays involve the use of semiconductors which absorb different amounts of energy depending on particle size. This energy is then re-emitted as photons of light. Different particle sizes give different colours.

Use band theory to explain why the larger particles produce colours toward the red end of the visible spectrum while smaller particles produce colours toward the violet end.





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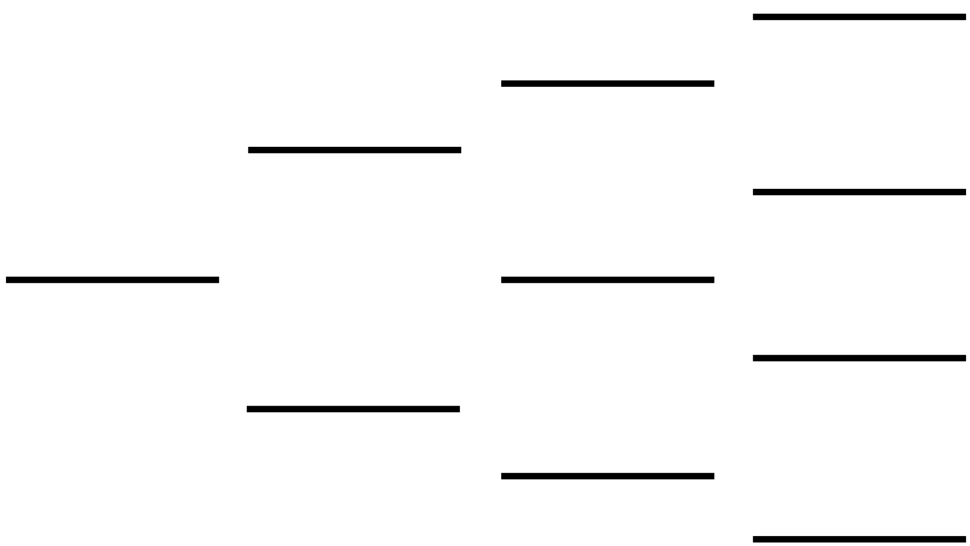
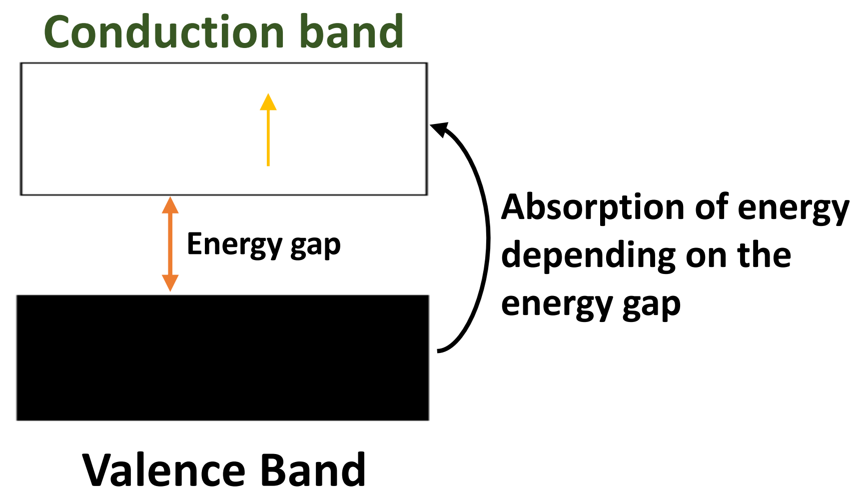
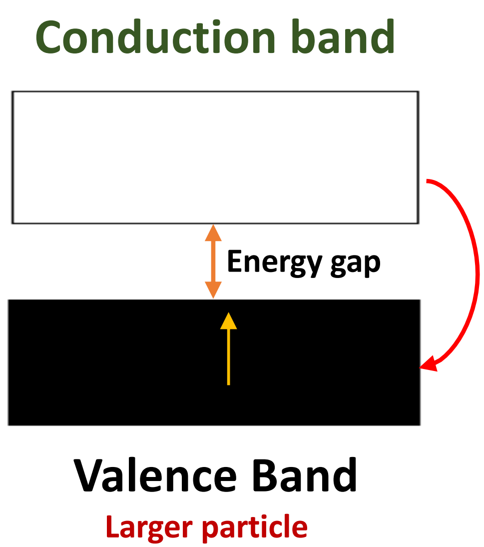
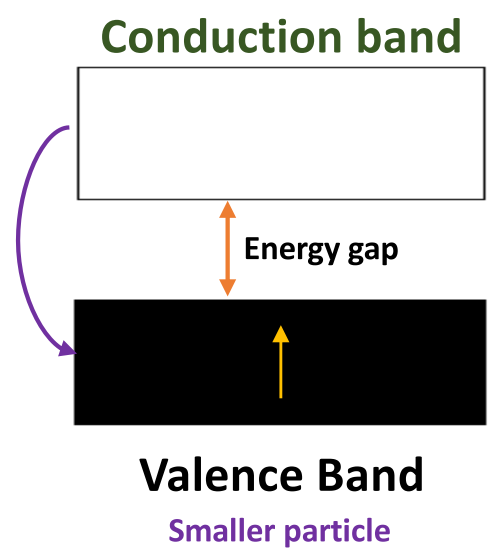


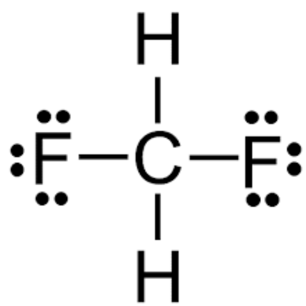




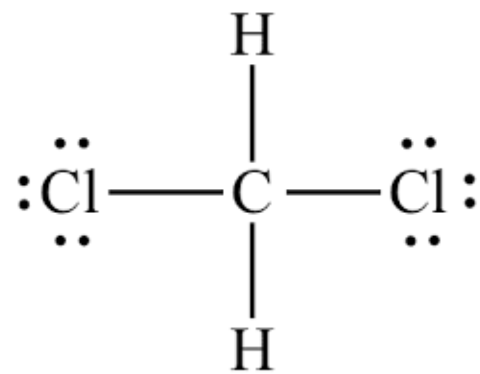
Emission of energy (photon), depending on absorbed energy.



CH_2F_2 has a boiling point of –52°C, while CH_2Cl_2 a boiling point of 40°C.
Why is the boiling point of dichloromethane 92° higher than that of difluoromethane?



Polar



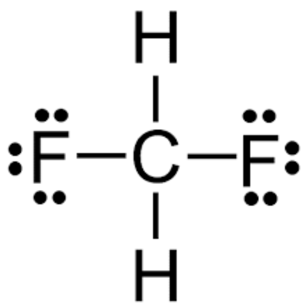
Polar

Fluorine more electronegative than Chlorine

It makes CH_2F_2 more polar than CH_2Cl_2.

But CH_2F_2 has lower boiling point than CH_2Cl_2?

CH_2F_2 has a boiling point of –52°C, while CH_2Cl_2 a boiling point of 40°C.
Why is the boiling point of dichloromethane 92° higher than that of difluoromethane?

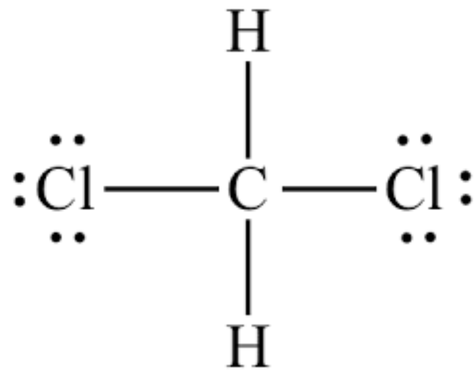


Polar

Dispersion forces

Dipole-dipole forces

Molar mass of CH_2F_2 = 52



Polar

Dispersion forces

Dipole-dipole forces

Molar mass of CH_2Cl_2 = 85

CH_2Cl_2 will have stronger dispersion forces than CH_2F_2

It leads to CH_2Cl_2 with higher boiling point than CH_2F_2