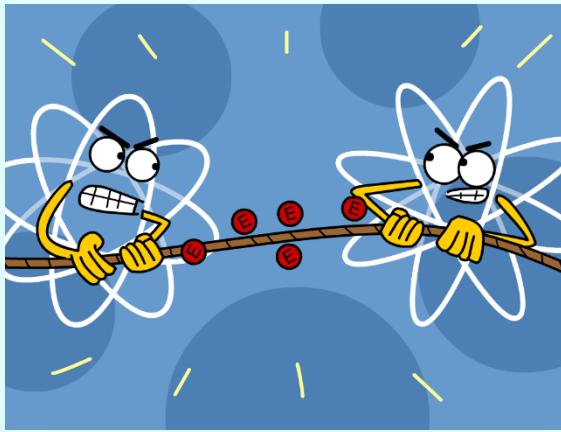


Chemical Bonding

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The contents of this presentation is made to provide a brief idea about the topic, details will be discussed in the classes. Contents have been collected from multiple textbooks and internet.

Chemical Bonding

- A **Chemical bond** is a force of attraction between atoms or ions.
- Atoms or ions are held together in molecules or compounds by chemical bonds.
- All chemical reactions involve breaking of some bonds and formation of new ones which yield new products with different properties.

Why do atoms form chemical bonds?

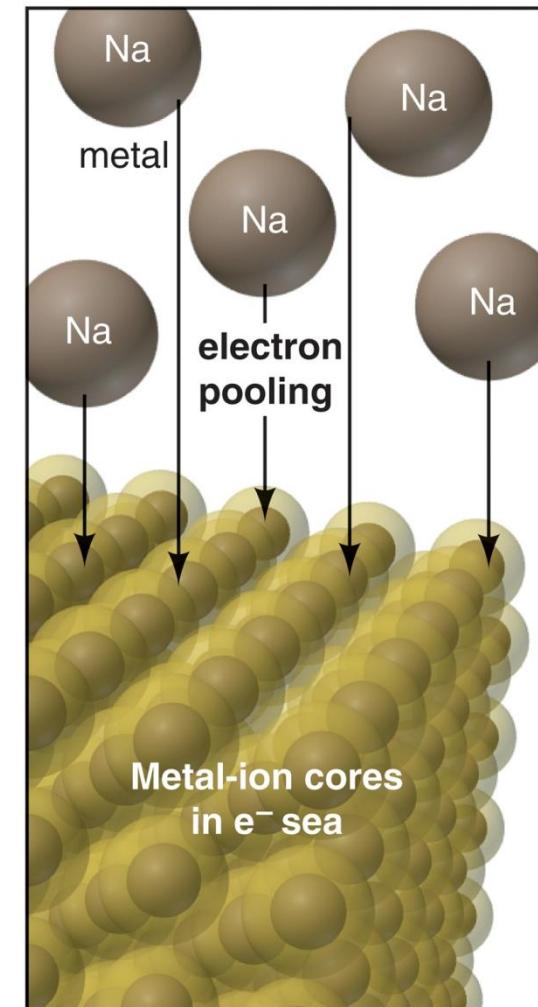
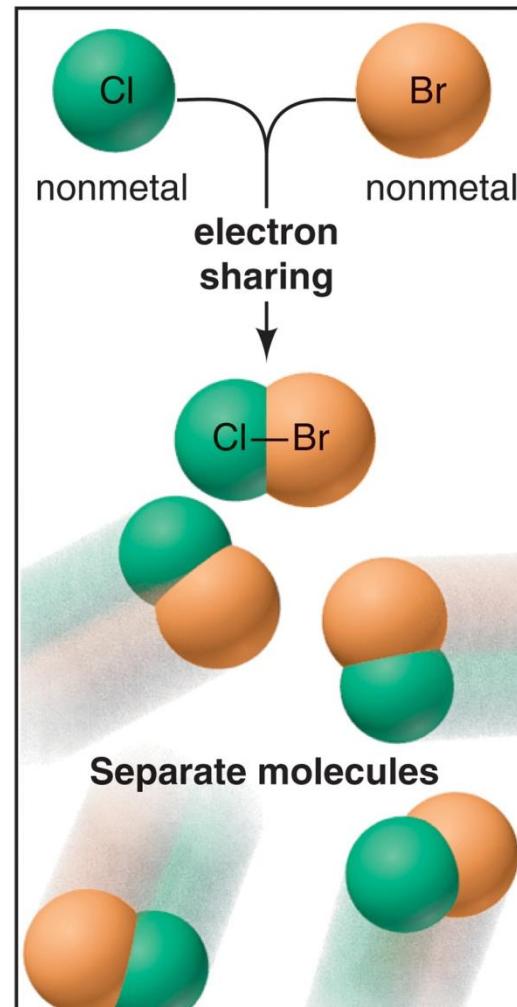
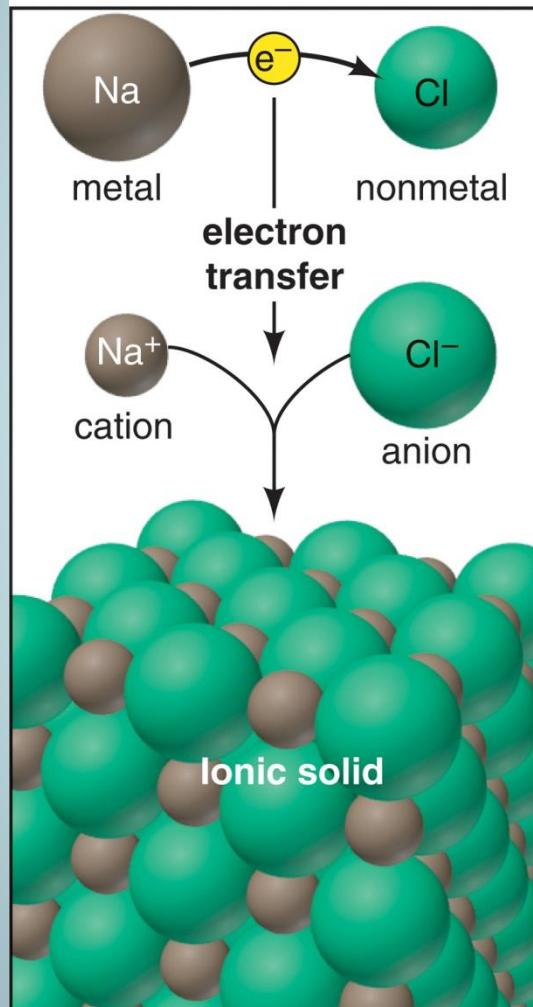
- To achieve a stable valence shell electron configuration of inert gases

Types of Chemical Bonding

- **Ionic bonding**
 - involves the **transfer** of electrons and is usually observed when a **metal** bonds to a **nonmetal**.
- **Covalent bonding**
 - involves the **sharing** of electrons and is usually observed when a **nonmetal** bonds to a **nonmetal**.
- **Metallic bonding**
 - involves **electron pooling** and occurs when a **metal** bonds to another **metal**.

More bonds: Co-ordination covalent bond, Hydrogen bond

Types of Chemical Bonding



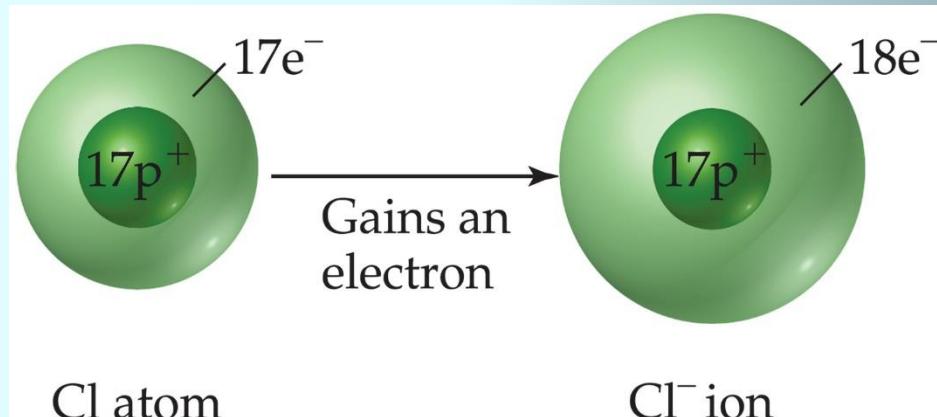
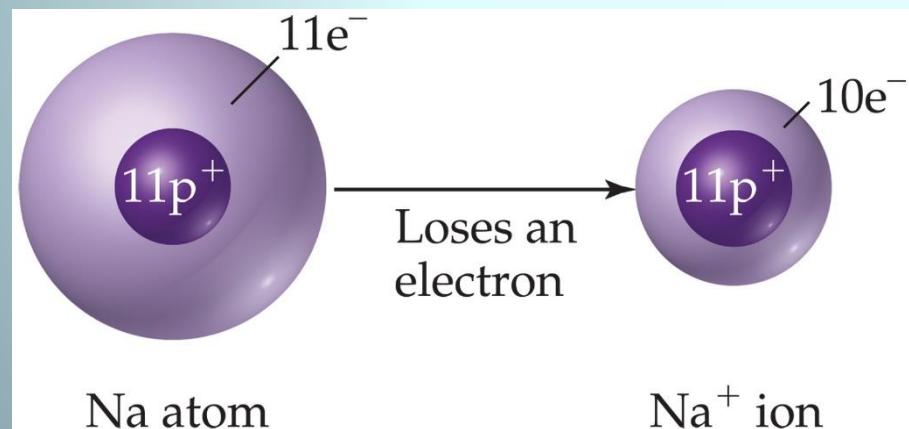
A Ionic bonding

B Covalent bonding

C Metallic bonding

Ionic Bonding

- An **ionic bond** is formed when a metal **transfers** electrons to a nonmetal to form **ions**, which attract each other to give a solid compound.
- The total number of electrons lost by the metal atom(s) equals the total number of electrons gained by the nonmetal atoms.

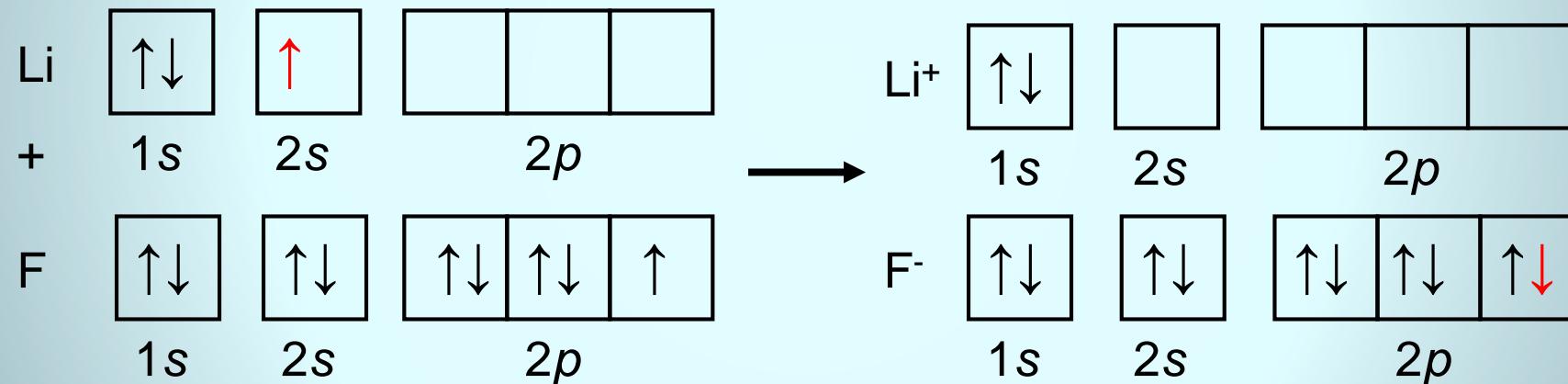


Ionic Bonding

Formation of ionic bonding between Li and F – through e⁻ configuration



Orbital diagrams

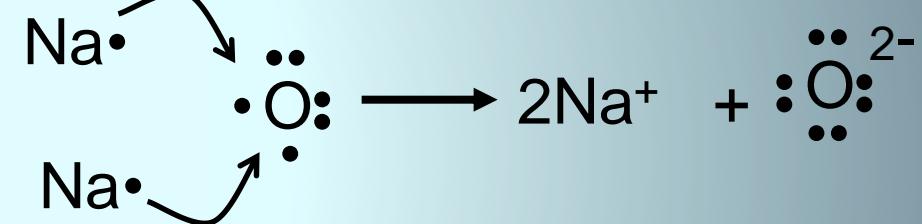
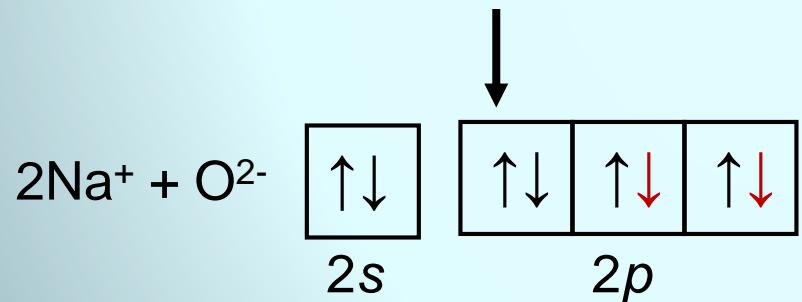
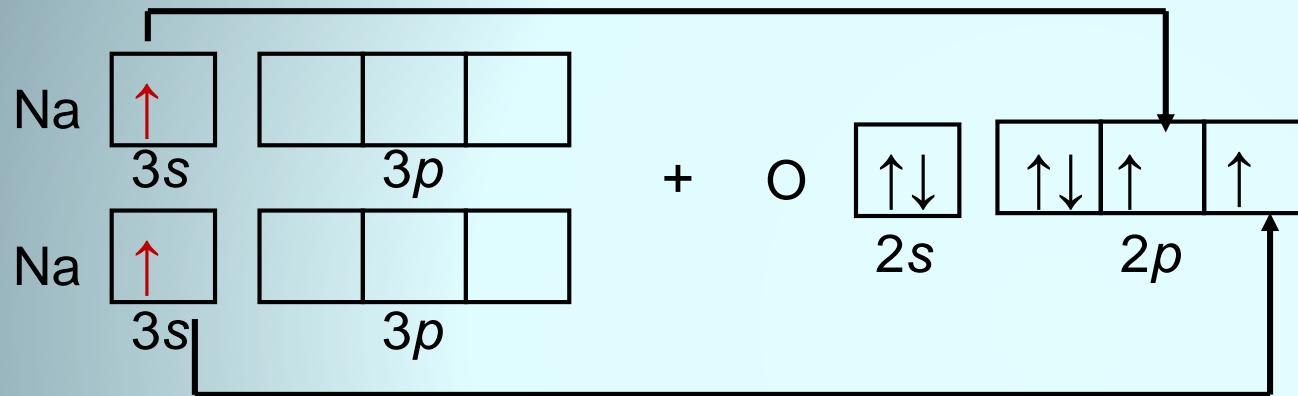


Lewis electron-dot symbols



Ionic Bonding

Formation of Na_2O



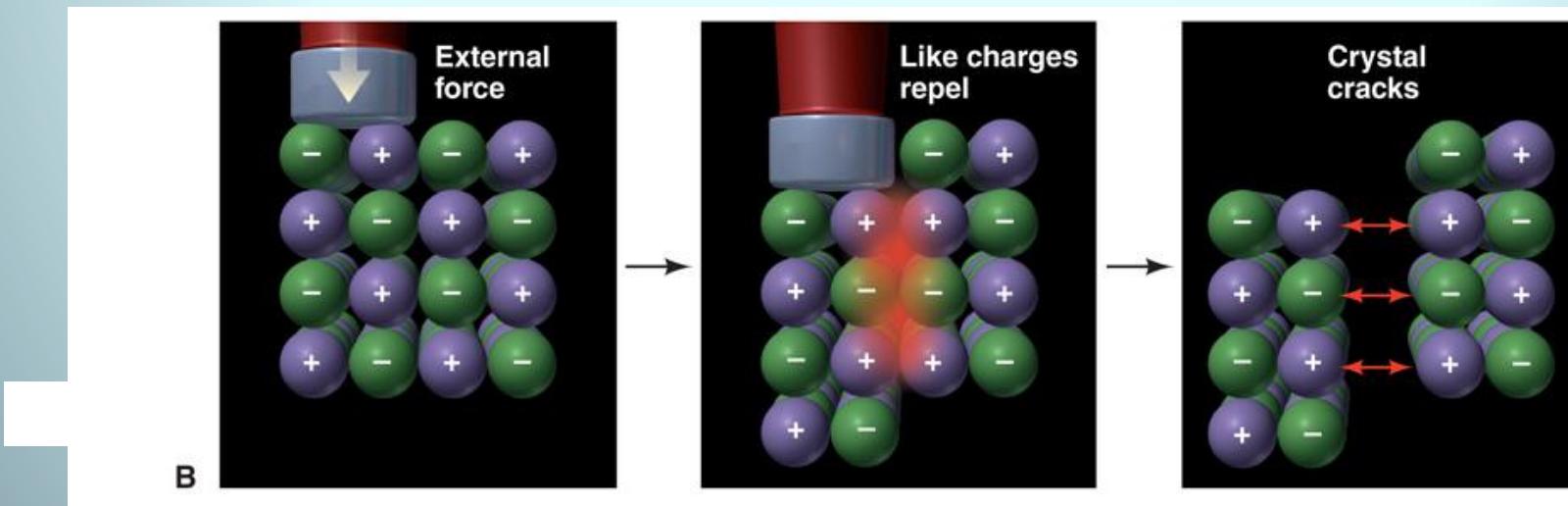
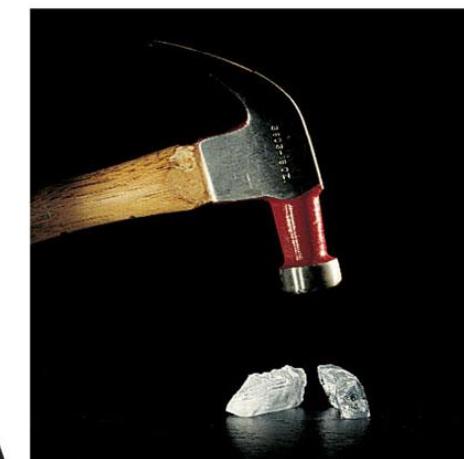
Ionic Bonding - Features

- Metal to nonmetal.
- Metal loses electrons to form cation.
- Nonmetal gains electrons to form anion.
- The electronegativity between the metal and the nonmetal must be greater than 2.
- Ionic bond results from + to – attraction.
 - Larger charge = stronger attraction.
 - Smaller ion = stronger attraction.

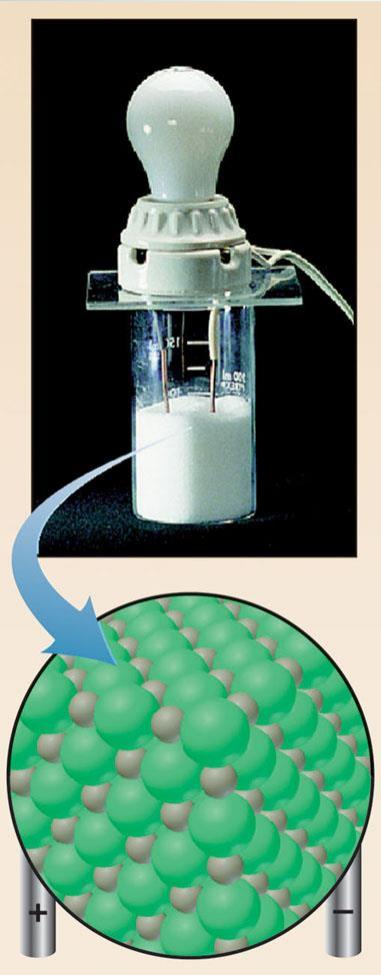
Properties of Ionic Compounds

- Ionic compounds tend to be hard, rigid, and brittle, with high melting points and boiling points.
- Ionic compounds do not conduct electricity in the solid state.
 - In the solid state, the ions are fixed in place in the lattice and do not move.
- Ionic compounds conduct electricity when melted or dissolved.
 - In the liquid state or in solution, the ions are free to move and carry a current.

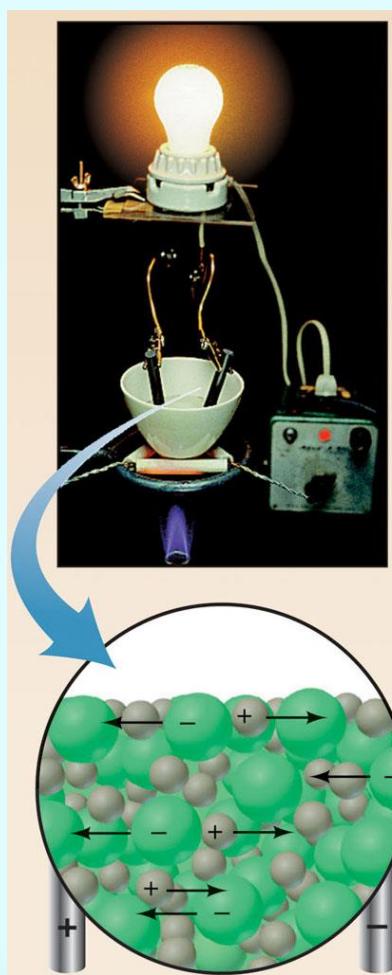
Why Ionic Compounds Crack?



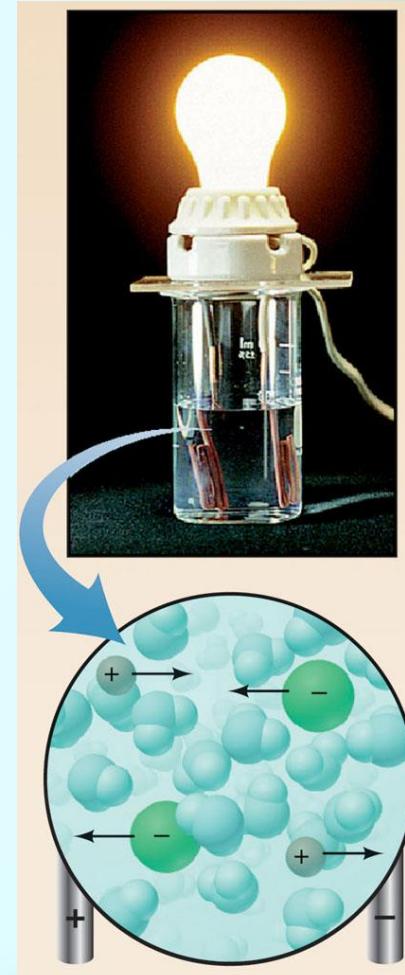
Electrical Conductance and Ion Mobility



Solid ionic compound



Molten ionic compound



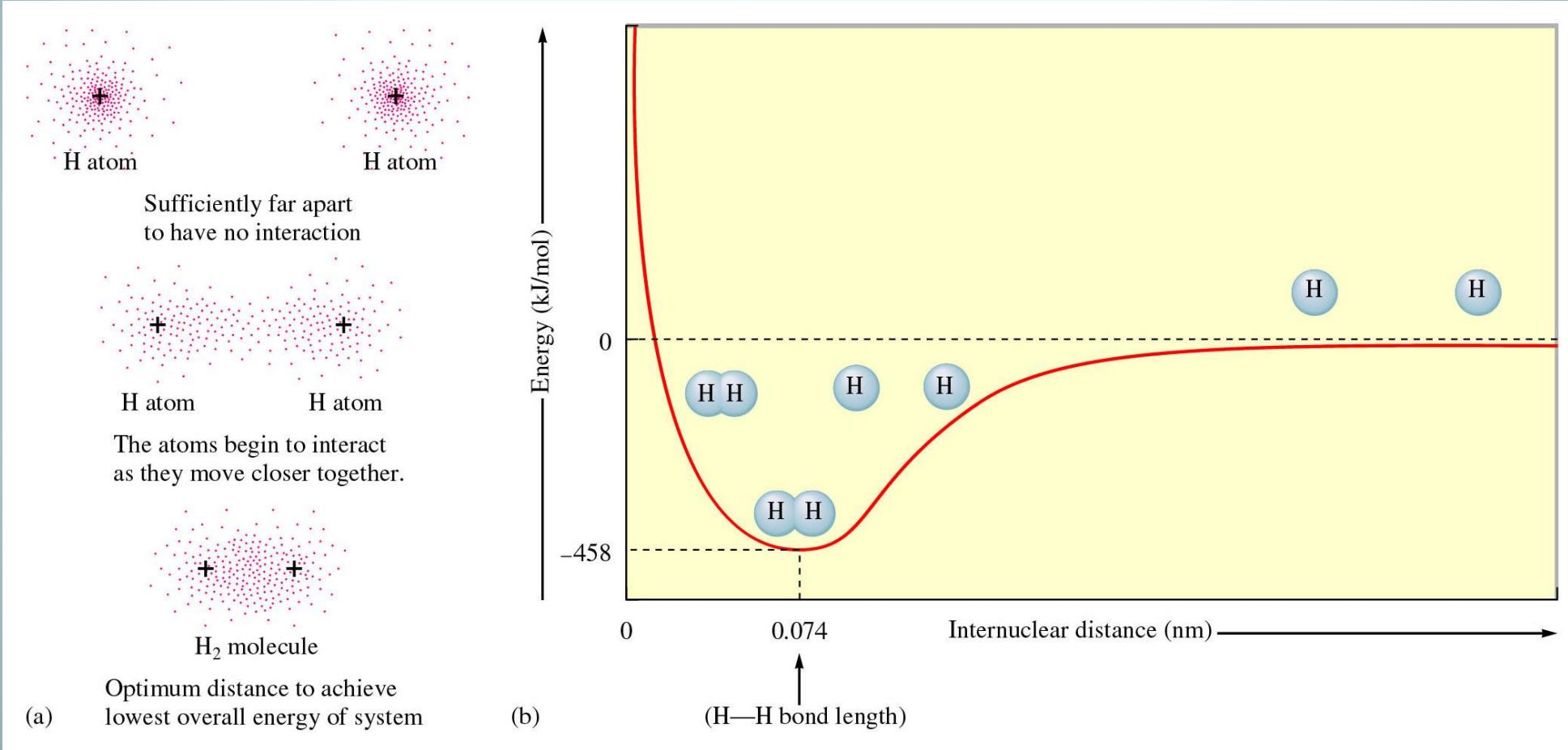
Ionic compound dissolved in water

Covalent Bonding

- Atoms **share** electrons to achieve a full outer level of electrons.
The shared electrons are called a **shared pair** or **bonding pair**.
- Often found between two **nonmetals**.
- Typical of molecular species.
- Atoms bonded together to form molecules.
- The shared pair is represented as a pair of dots or a line:

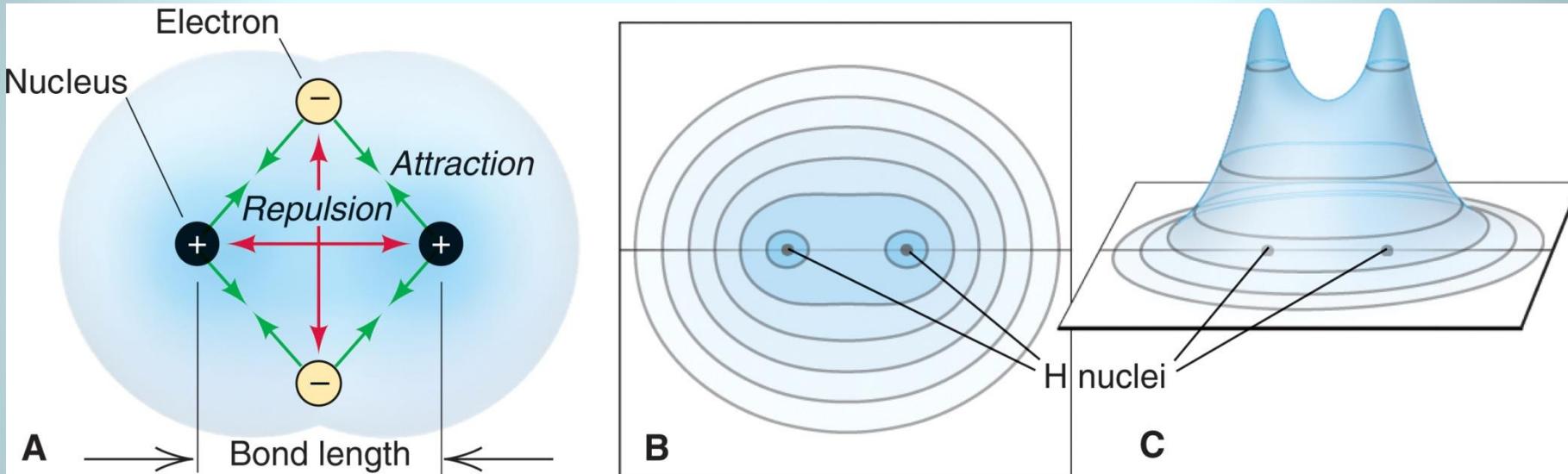


Covalent Bonding



Covalent Bonding

Distribution of electron density in H₂.



At some distance (bond length), attractions balance repulsions.

Electron density is high around and between the nuclei.

Covalent Bonding

The **bond order** is the number of electron pairs being shared by a given pair of atoms. A single bond consists of one bonding pair and has a bond order of 1.

The **bond energy** (BE) is the energy needed to overcome the attraction between the nuclei and the shared electrons. The **stronger** the bond the **higher** the bond energy.

The **bond length** is the distance between the nuclei of the bonded atoms.

Covalent Bonding

For a given pair of atoms, a ***higher bond order*** results in a ***shorter bond length*** and ***higher bond energy***.

For a given pair of atoms, a ***shorter bond*** is a ***stronger bond***.

Bond length ***increases*** down a group in the periodic table and ***decreases*** across the period. Bond energy shows the opposite trend.

Covalent Bonding

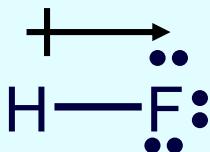
Table Average Bond Energies (kJ/mol) and Bond Lengths (pm)

Electronegativity and Bond Polarity

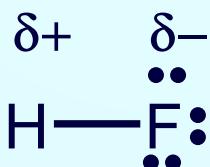
- A covalent bond in which the shared electron pair is not shared equally, but remains closer to one atom than the other, is a **polar covalent bond**.
- The ability of an atom in a covalent bond to attract the shared electron pair is called its **electronegativity**.
- Unequal sharing of electrons causes the more electronegative atom of the bond to be *partially negative* and the less electronegative atom to be *partially positive*.

Electronegativity and Bond Polarity

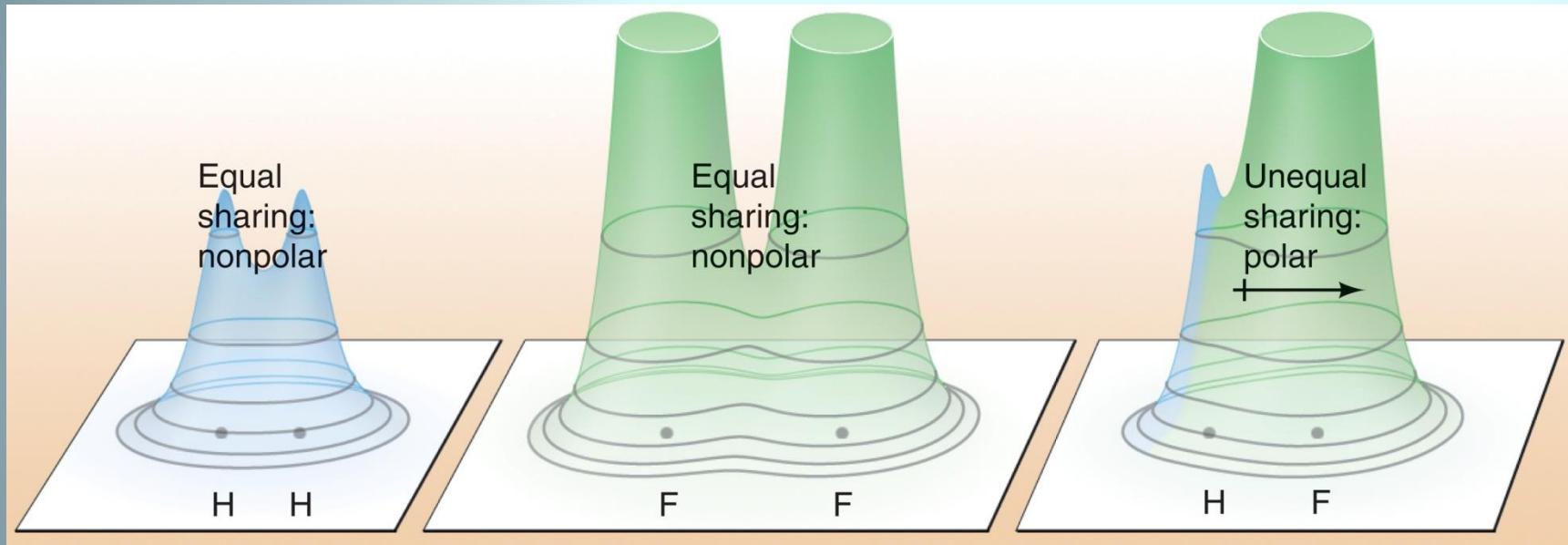
The unequal sharing of electrons can be depicted by a polar arrow. The head of the arrow points to the *more electronegative element*.



A polar bond can also be marked using $\delta+$ and $\delta-$ symbols.



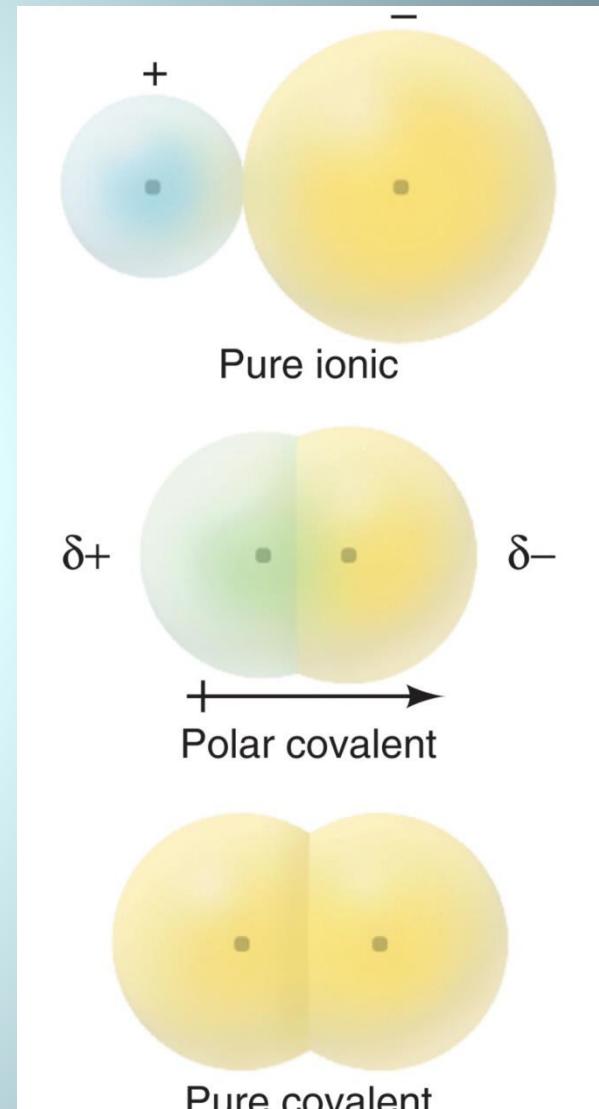
Electronegativity and Bond Polarity



Electron density distributions in H₂, F₂, and HF

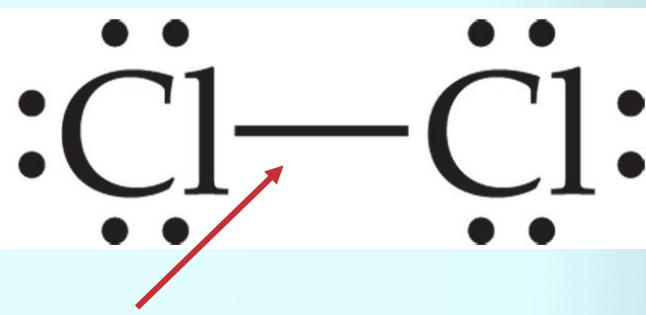
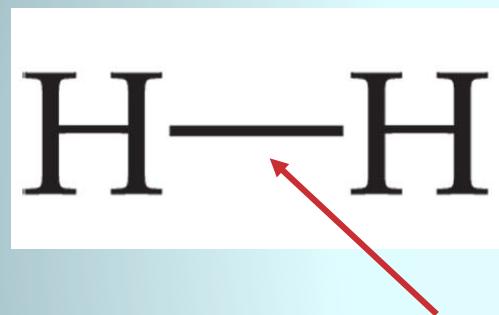
In HF, the electron density shifts from H to F.

The H–F bond has partial ionic character.



Lewis Structures

Lewis structures are representations of molecules showing all valence electrons, bonding and nonbonding.

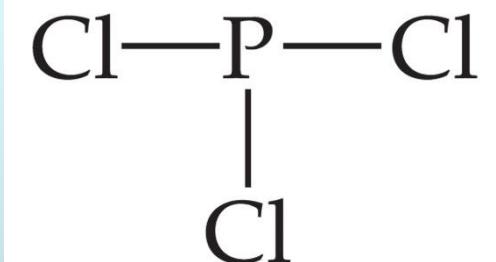
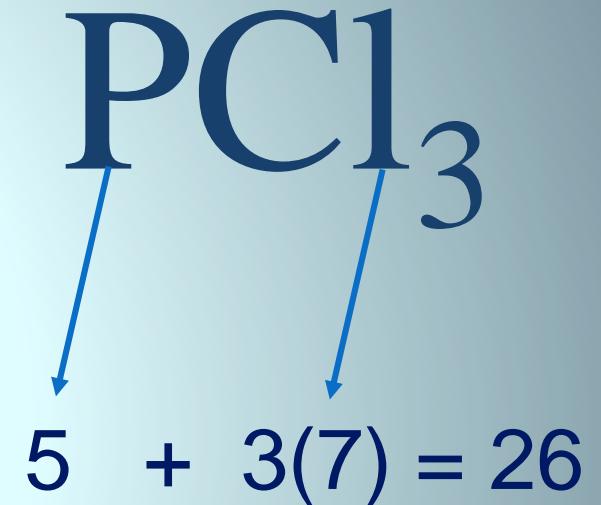


Lines correspond to 2 electrons in bond

Drawing Lewis Structures

A way to keep track of those valence electrons

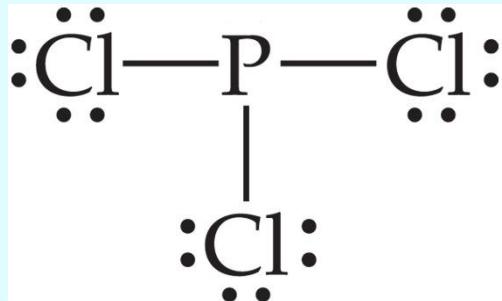
1. Find the sum of valence electrons of all atoms in the polyatomic ion or molecule.
 - If it is an anion, add one electron for each negative charge.
 - If it is a cation, subtract one electron for each positive charge.
2. The central atom is the *least* electronegative element. Connect the outer atoms to it by single bonds.



Keep track of the electrons:
 $26 - 6 = 20$

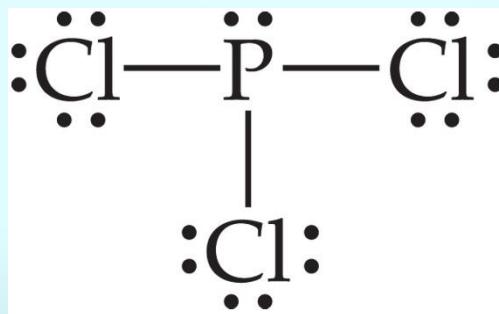
Drawing Lewis Structures

3. Put eight electrons around the outer atoms (“fill their octet”)



Keep track of the electrons:
 $26 - 6 = 20 - 18 = 2$

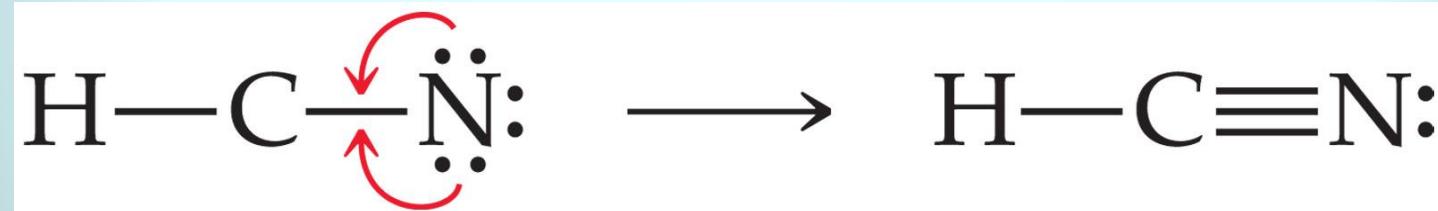
4. Fill the octet of the central atom.



Keep track of the electrons:
 $26 - 6 = 20 - 18 = 2 - 2 = 0$

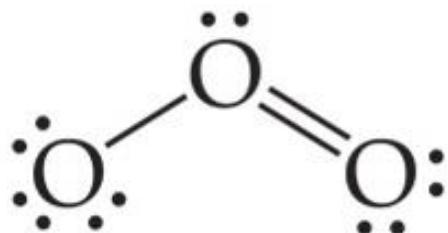
Drawing Lewis Structures

5. If you run out of electrons before the central atom has an octet, form multiple bonds until it does.



Resonance

Lets draw the Lewis structure for ozone, O₃.

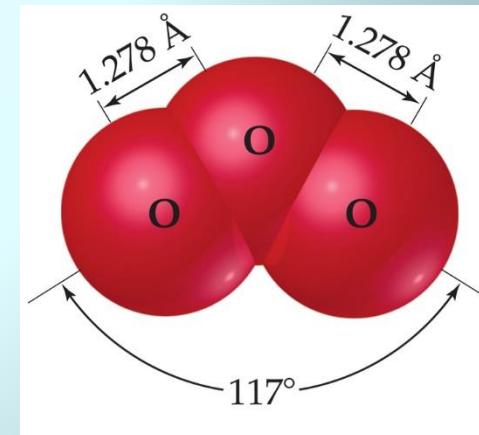


But why should one O be different from the other?

In actual structure of O₃

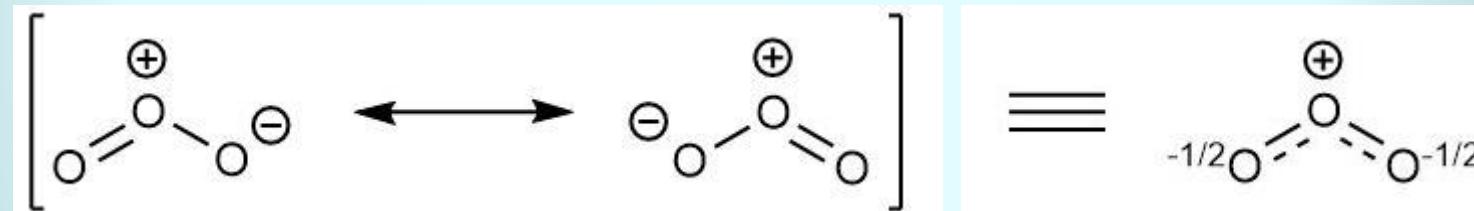
...both O—O bonds are the same length.

...both outer oxygens have a charge of -1/2.

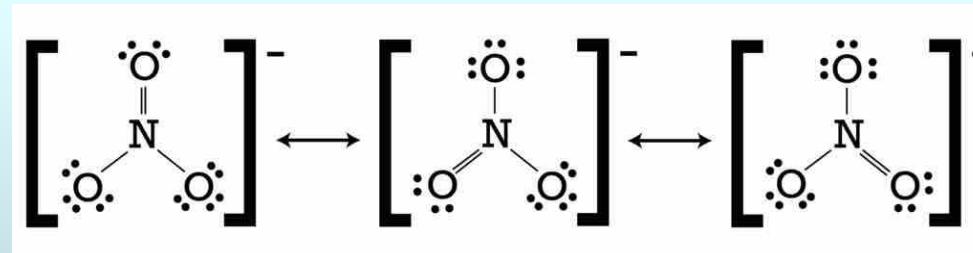


Resonance

- One Lewis structure cannot accurately depict a molecule such as ozone.
- We use multiple structures, resonance structures, to describe the molecule.



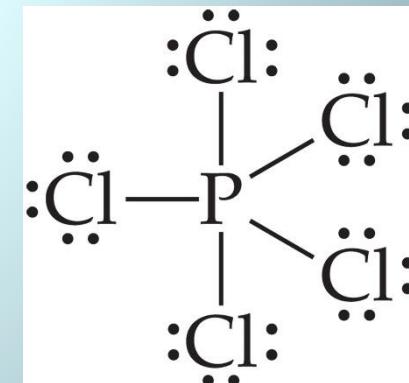
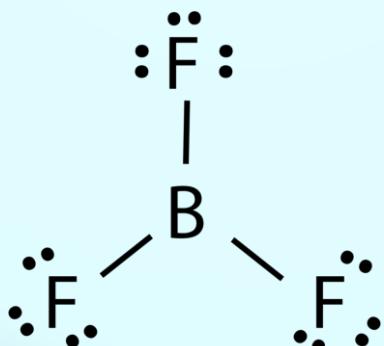
- Resonance structure of NO_3^-



Resonance

Exceptions to the Octet Rule

- There are three types of ions or molecules that do not follow the octet rule:
 - Ions or molecules with an odd number of electrons.
 - Ions or molecules with less than an octet.
 - Ions or molecules with more than eight valence electrons (an expanded octet).



Theories of Covalent Bonding

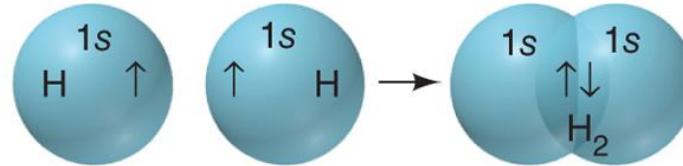
1. Valence Bond Theory (VBT)

The basic principle of VB theory:

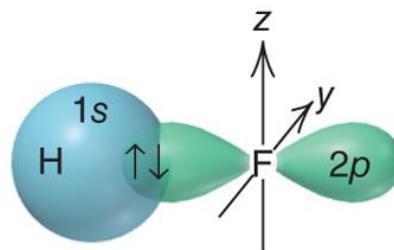
- A covalent bond forms when the orbitals of two atoms *overlap* and a pair of electrons occupy the overlap region.
- The space formed by the overlapping orbitals can accommodate a *maximum of two electrons* and these electrons must have *opposite (paired) spins*.
- The greater the orbital overlap, the stronger the bond. Extent of orbital overlap depends on orbital shape and direction.
- The orbitals that form when bonding occurs are *different* from the atomic orbitals in the isolated atoms.

Valence Bond Theory

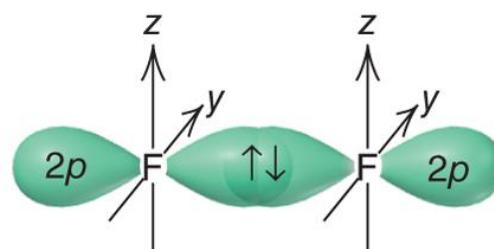
Orbital orientation and maximum overlap.



A Hydrogen, H_2



B Hydrogen fluoride, HF



C Fluorine, F_2

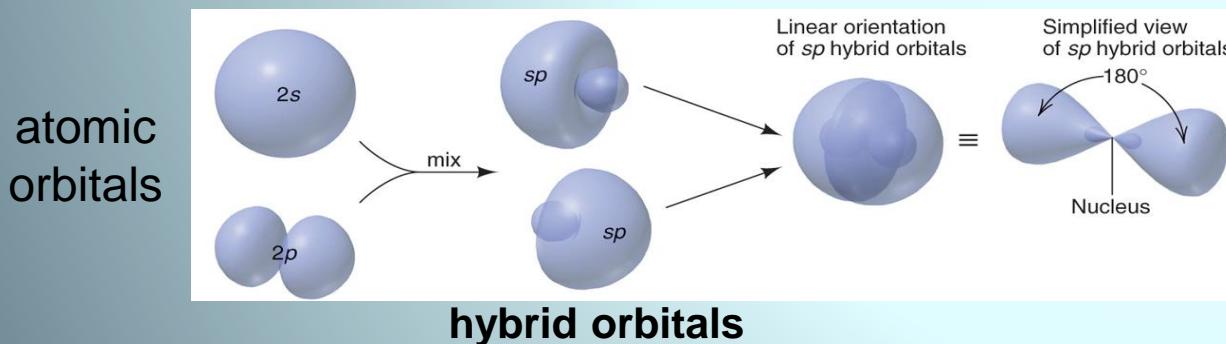
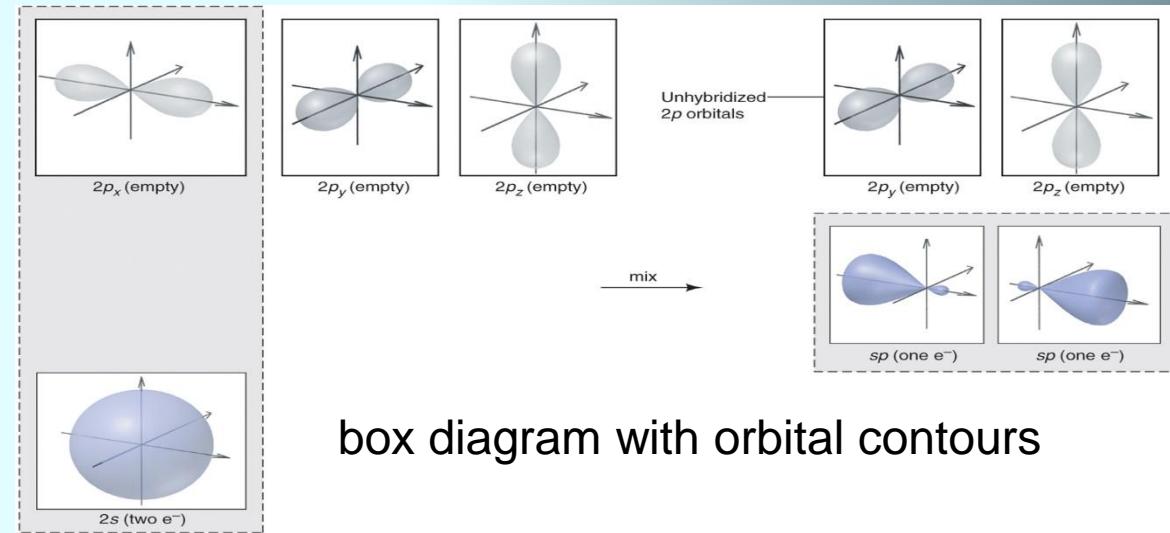
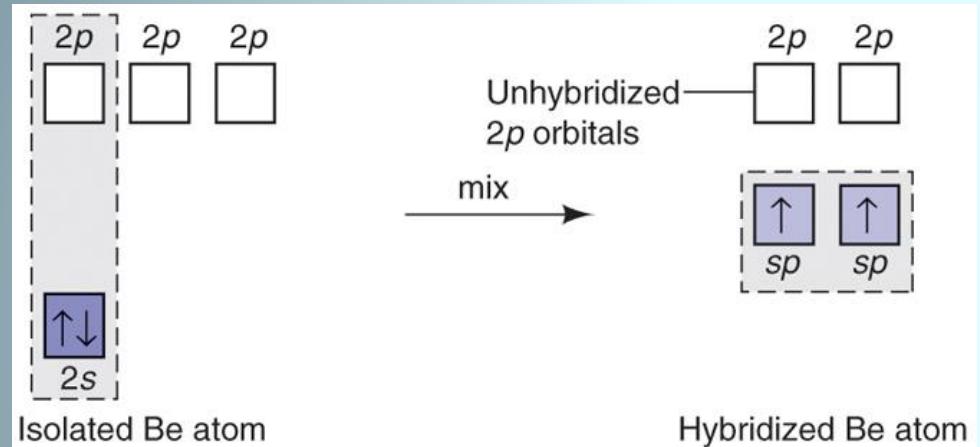
Valence Bond Theory

Hybridization

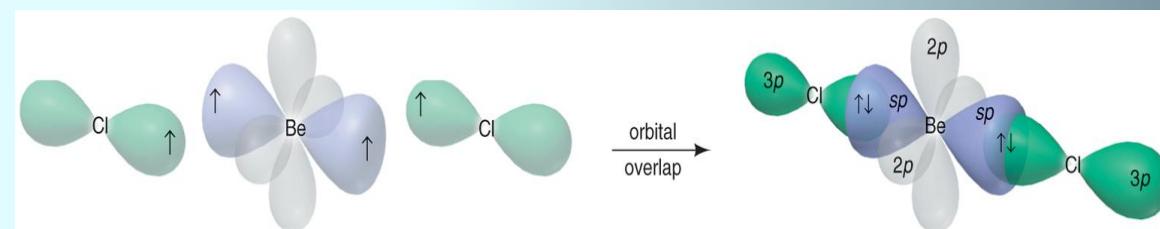
- Mixing of different types of atomic orbitals to form a uniform set of hybrid orbitals.
- The energy of the hybrid orbitals are different than the atomic orbitals.
- The number of hybrid orbitals formed equals the number of atomic orbitals mixed.
- The type of hybrid orbitals formed varies with the types of atomic orbitals mixed.
- The shape and orientation of a hybrid orbital maximizes overlap with the other atom in the bond.

Hybridization

Formation and orientation of *sp* hybrid orbitals and the bonding in BeCl₂.



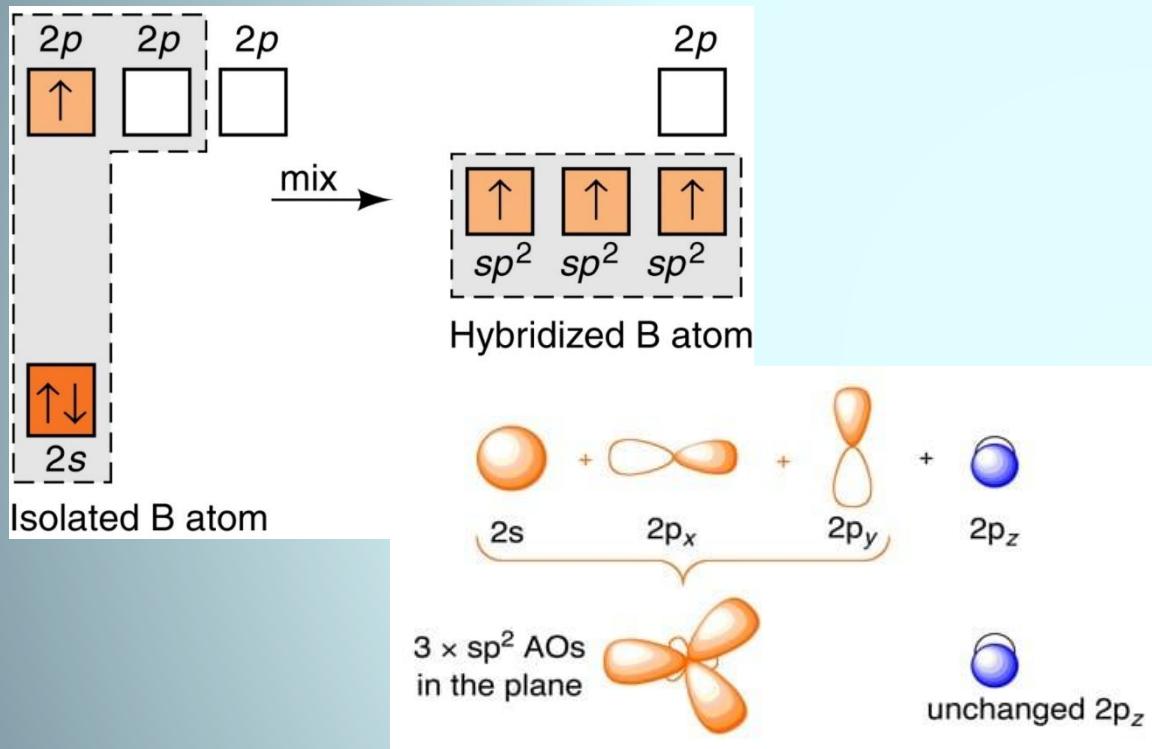
One 2s and one 2p atomic orbital mix to form two *sp* hybrid orbitals.



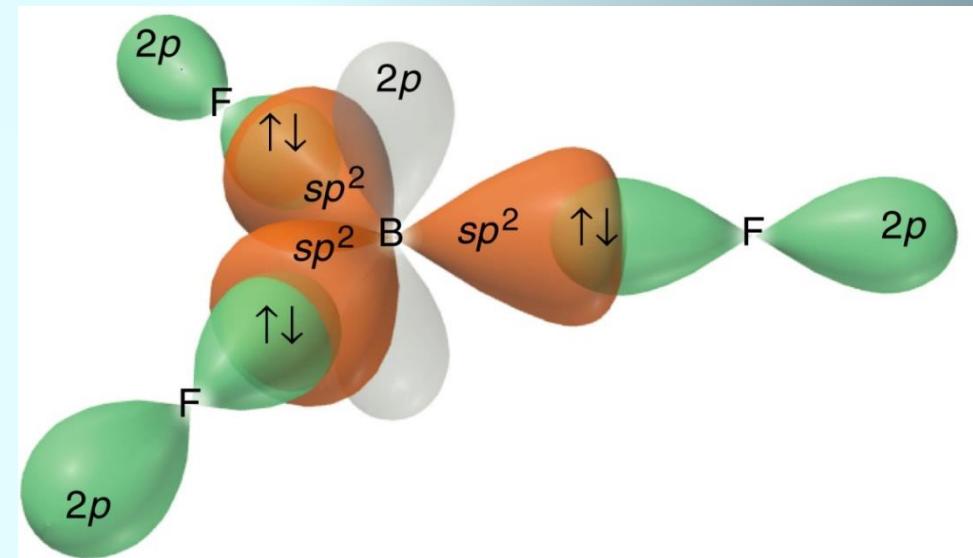
Overlap of Be and Cl orbitals to form BeCl₂.

Hybridization

The sp^2 hybrid orbitals in BF_3



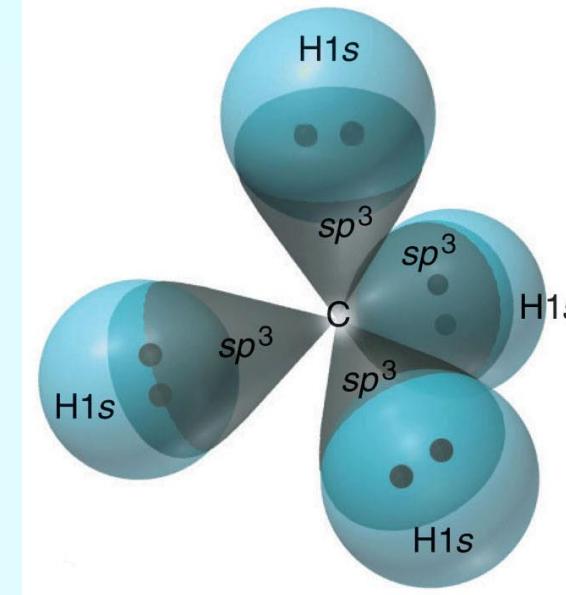
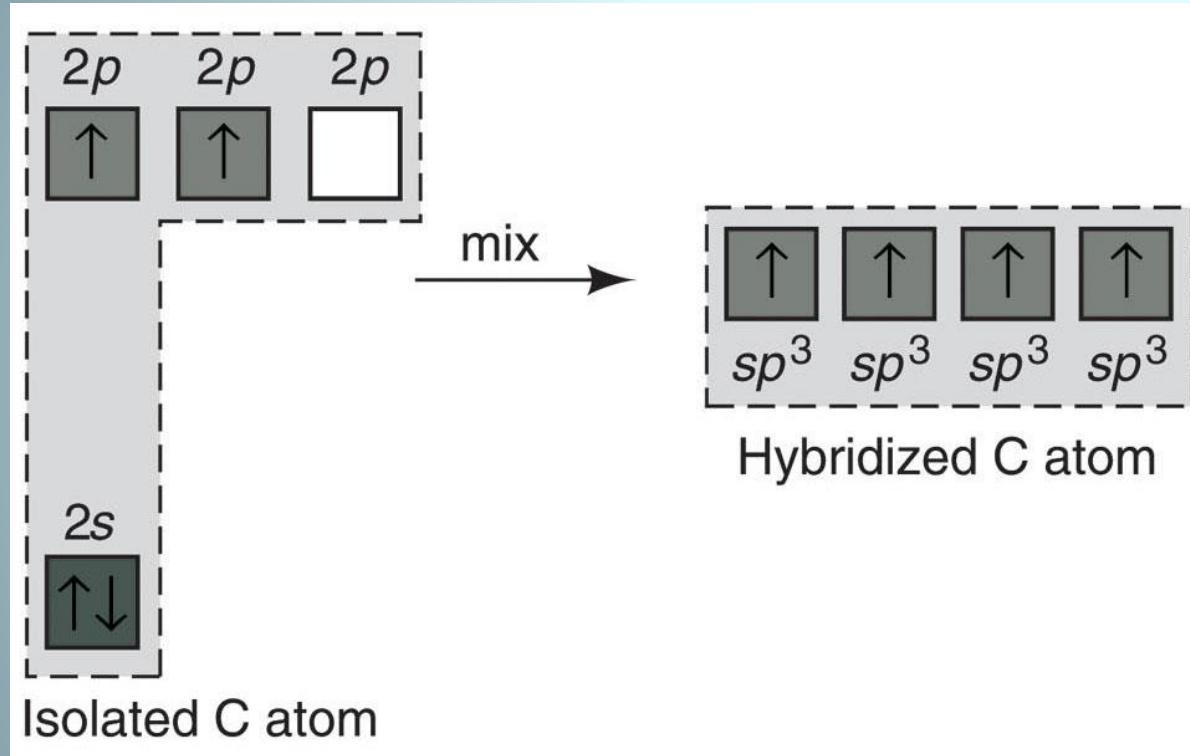
- ✓ Mixing one s and two p orbitals gives three sp^2 hybrid orbitals. The third $2p$ orbital remains unhybridized.



- ✓ The three sp^2 orbitals point to the corners of an equilateral triangle, their axes 120° apart.
- ✓ Each half-filled sp^2 orbital overlaps with the half-filled $2p$ orbital of a F atom.

Hybridization

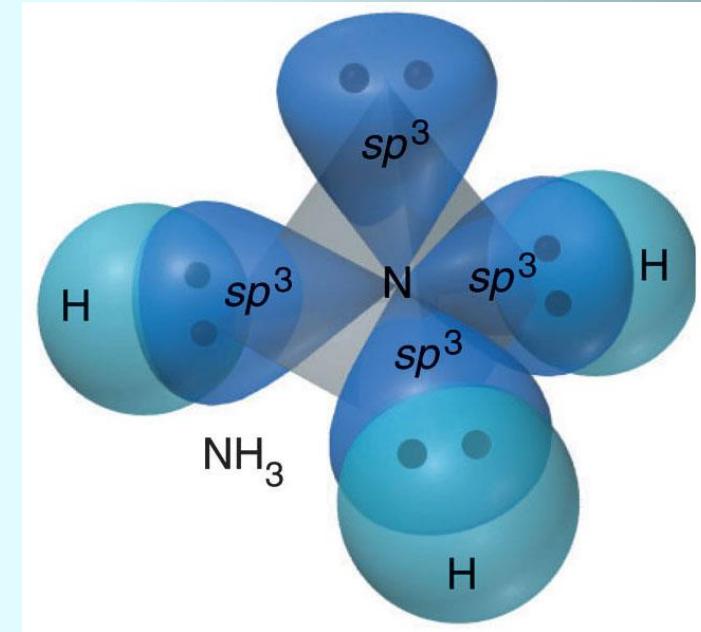
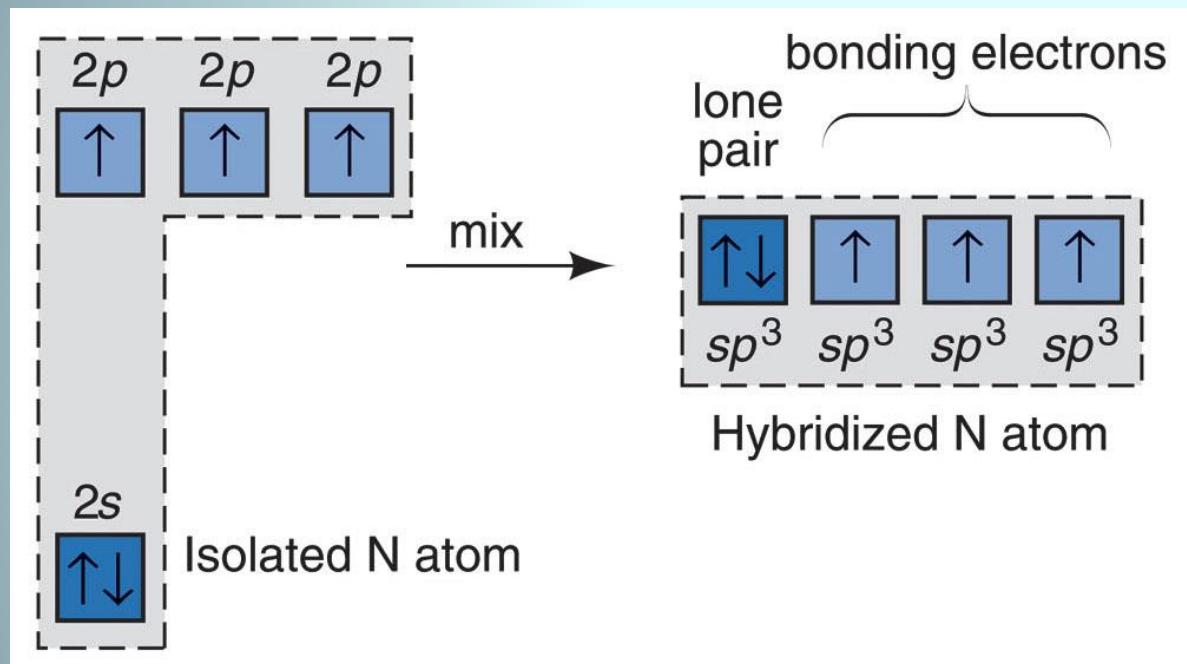
The sp^3 hybrid orbitals in CH_4



The four sp^3 orbitals adopt a tetrahedral shape

Hybridization

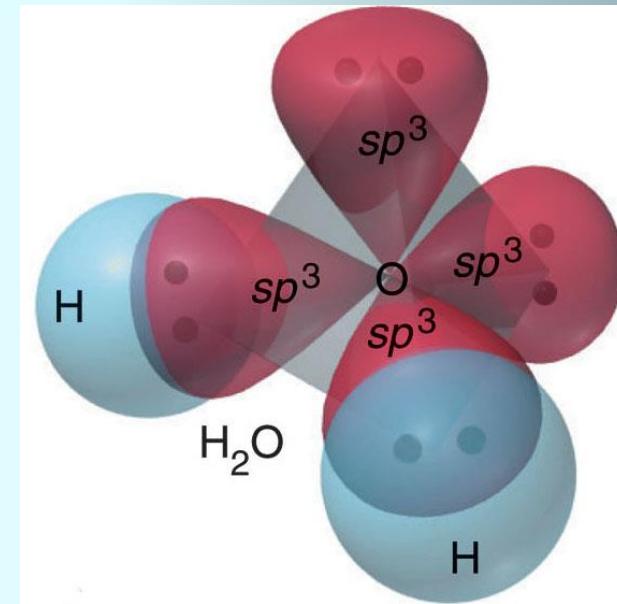
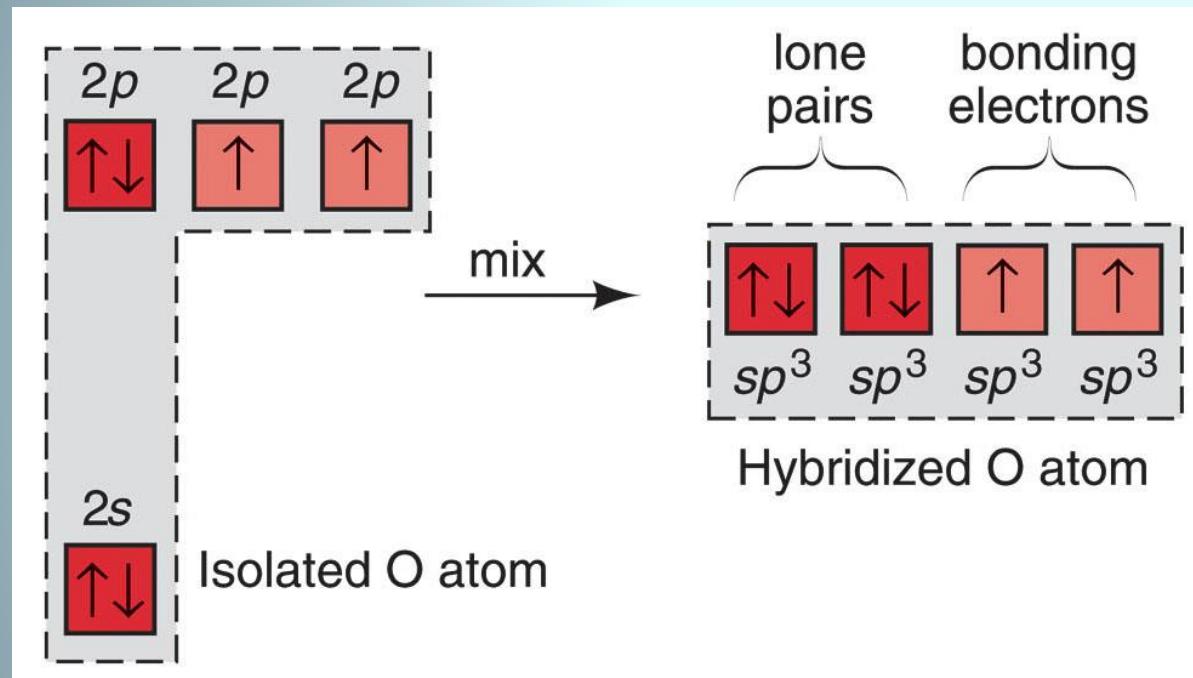
The sp^3 hybrid orbitals in NH_3



The N lone pair occupies an sp^3 hybrid orbital, giving a trigonal pyramidal shape.

Hybridization

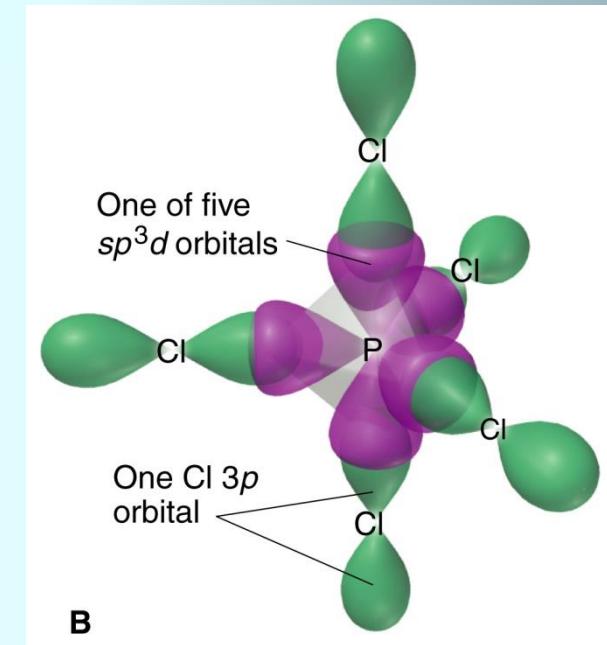
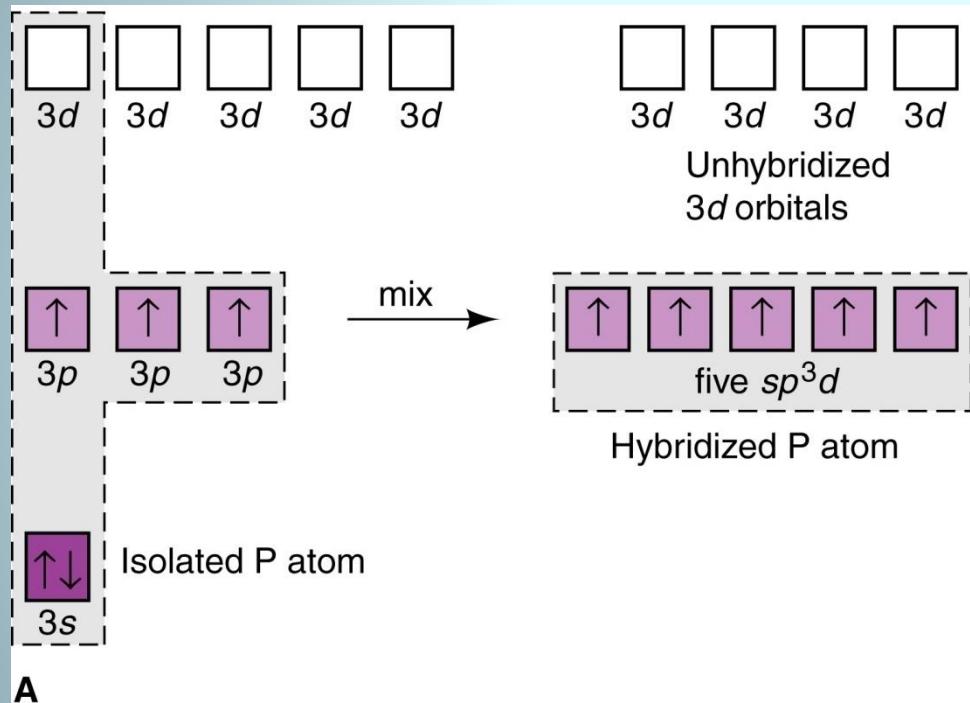
The sp^3 hybrid orbitals in H_2O



The O lone pairs occupy sp^3 hybrid orbitals, giving a bent shape.

Hybridization

The sp^3d hybrid orbitals in PCl_5



The formation of more than four bonding orbitals requires *d* orbital involvement in hybridization.

Hybridization

The sp^3d^2 hybrid orbitals in SF_6

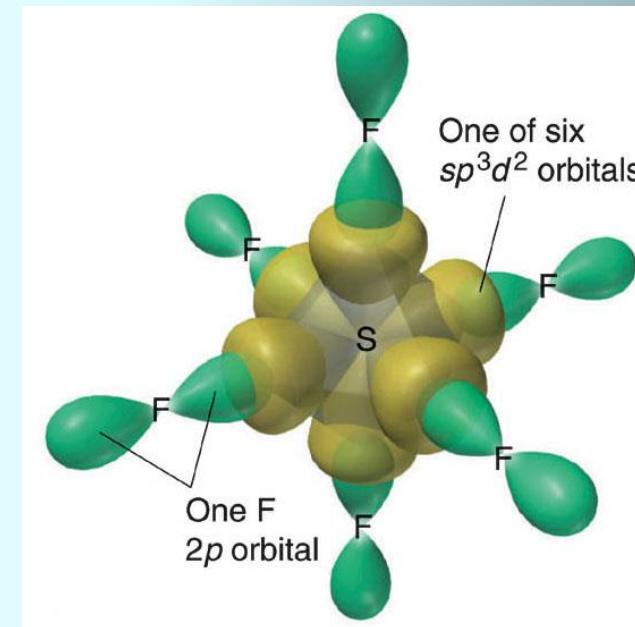
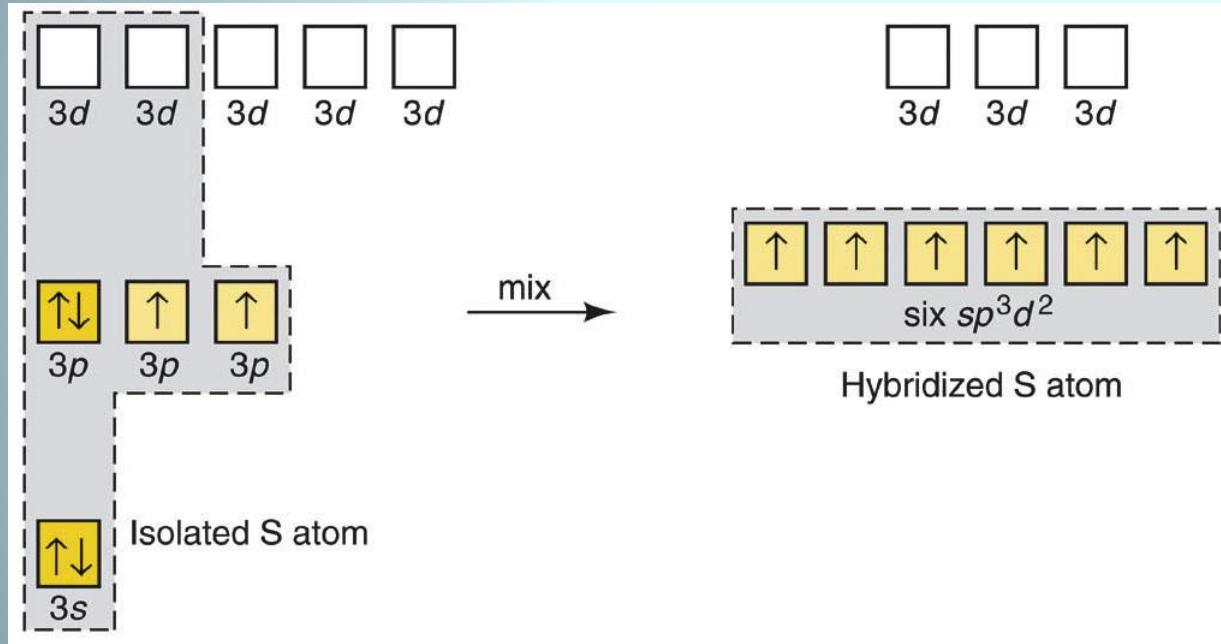
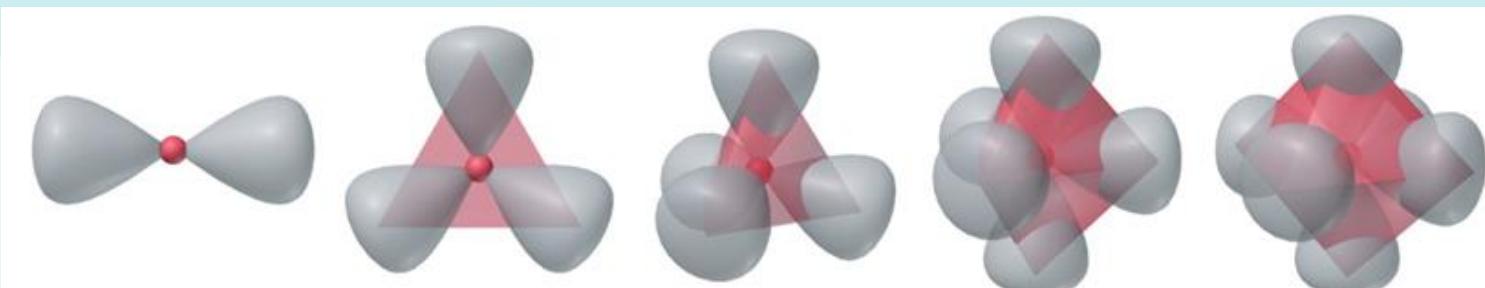


Table 11.1 Composition and Orientation of Hybrid Orbitals

	Linear	Trigonal Planar	Tetrahedral	Trigonal Bipyramidal	Octahedral
Atomic orbitals mixed	one s one <i>p</i>	one s two <i>p</i>	one s three <i>p</i>	one s three <i>p</i> one <i>d</i>	one s three <i>p</i> two <i>d</i>
Hybrid orbitals formed	two <i>sp</i>	three <i>sp</i> ²	four <i>sp</i> ³	five <i>sp</i> ³ <i>d</i>	six <i>sp</i> ³ <i>d</i> ²
Unhybridized orbitals remaining	two <i>p</i>	one <i>p</i>	none	four <i>d</i>	three <i>d</i>
Orientation					

Types of Covalent Bonds

▪ Sigma (σ) bond

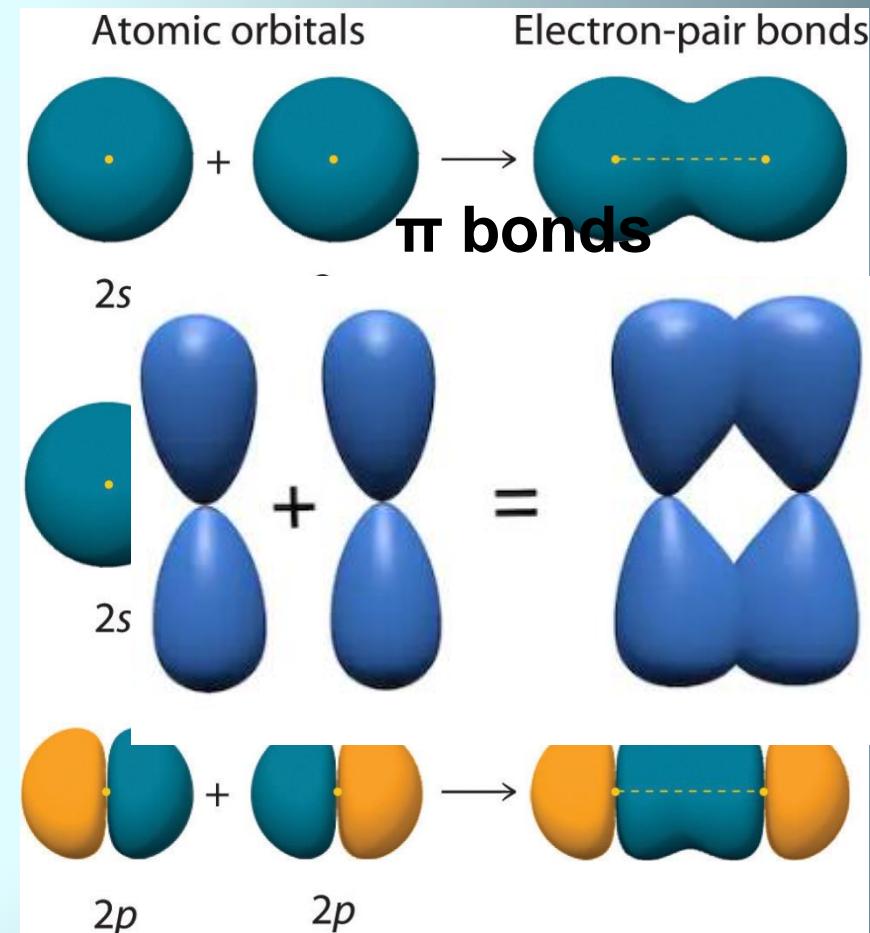
when the bonding orbitals point along the axis connecting the two bonding nuclei, by **head to head** overlapping

- either standard atomic orbitals or hybrids
 - s-to-s, p-to-p, hybrid-to-hybrid, s-to-hybrid, etc.
- All single bonds are σ bonds

▪ Pi (π) bond

- when the bonding orbitals are parallel to each other and perpendicular to the axis connecting the two bonding nuclei, by **sideways** overlapping
 - between unhybridized parallel p orbitals

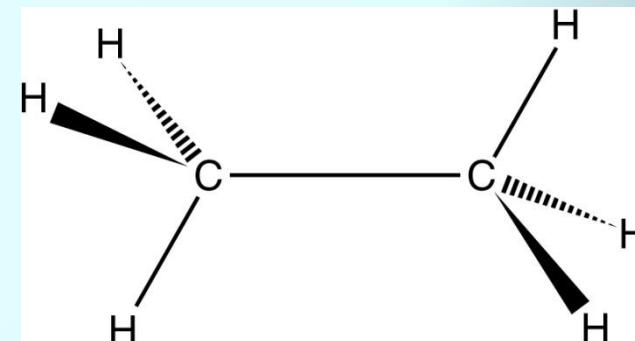
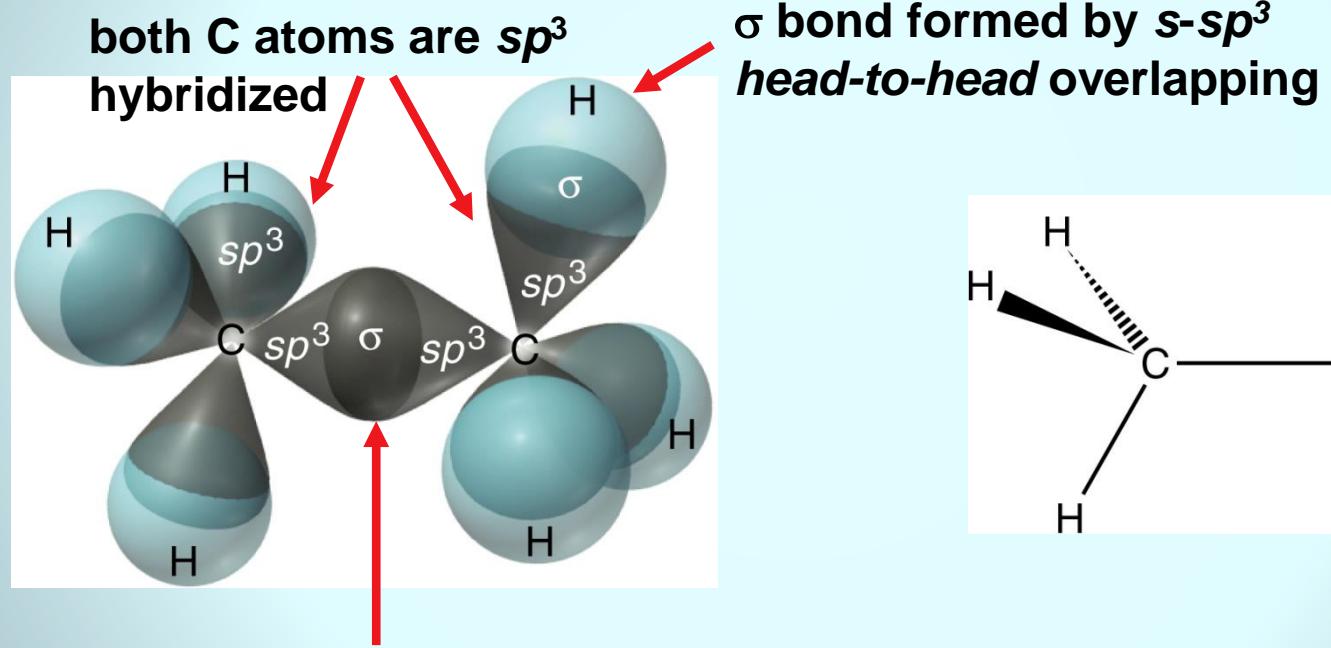
σ bonds



A π bond is weaker than a σ bond because sideways overlap is less effective than end-to-end overlap

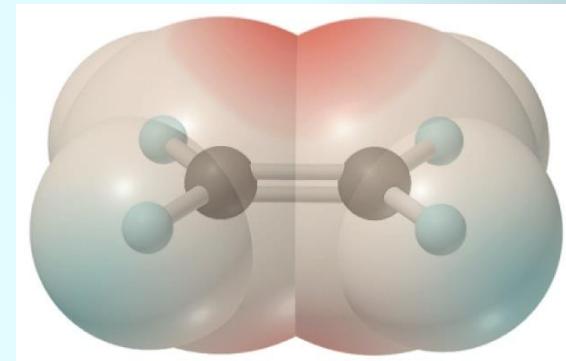
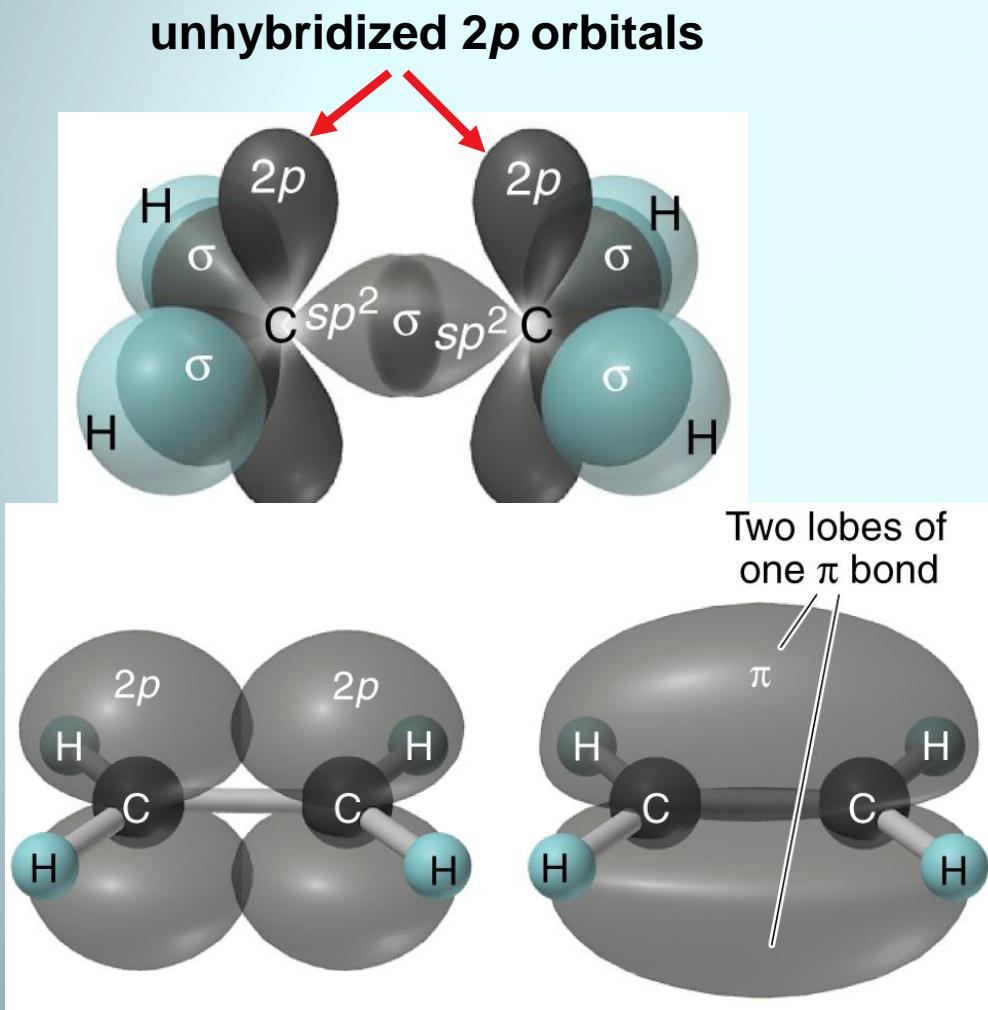
Types of Covalent Bonds

The σ bonds in ethane (C_2H_6).

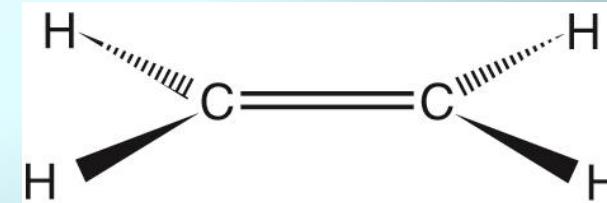


Types of Covalent Bonds

The σ and π bonds in ethylene (C_2H_4).

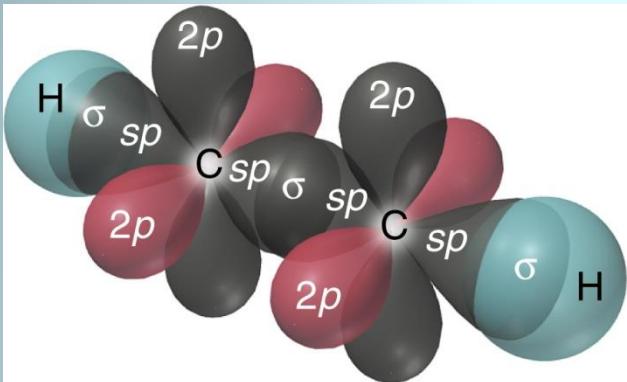


A π bond has two regions of electron density.

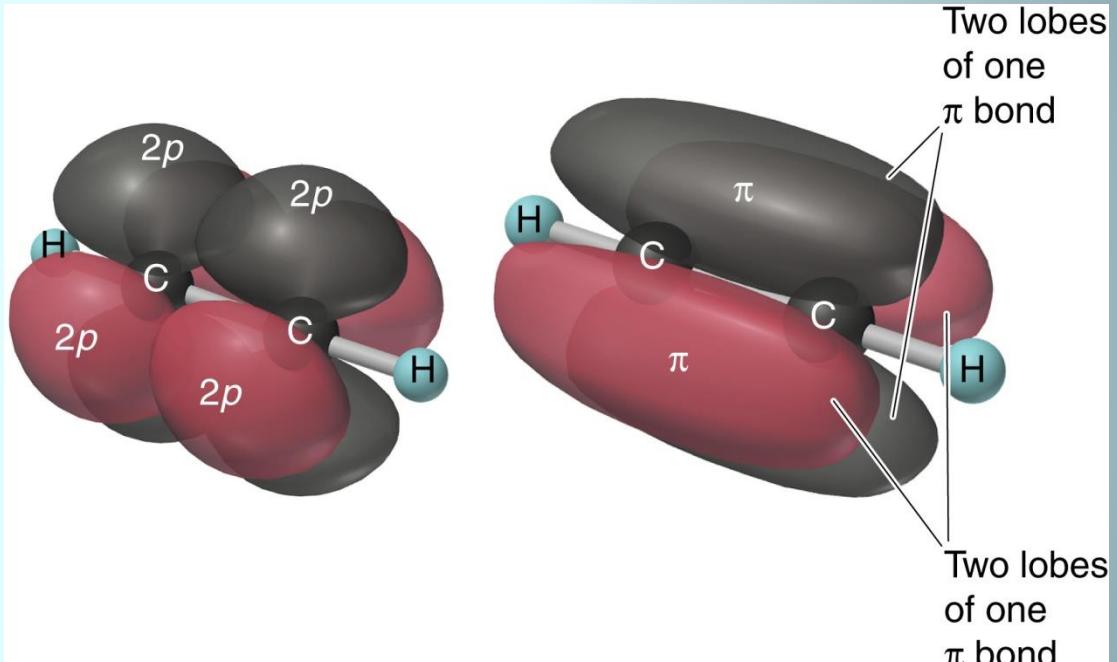
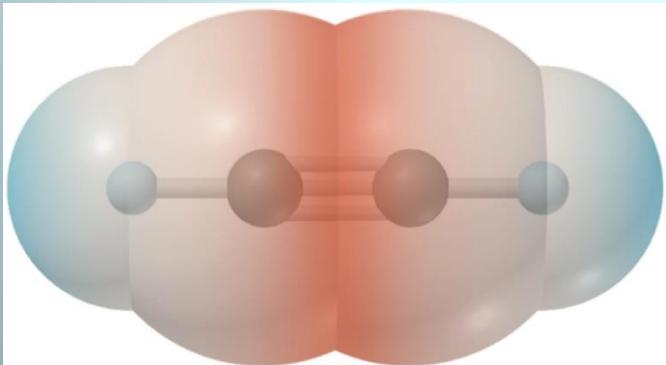


Types of Covalent Bonds

The σ and π bonds in acetylene (C_2H_2).



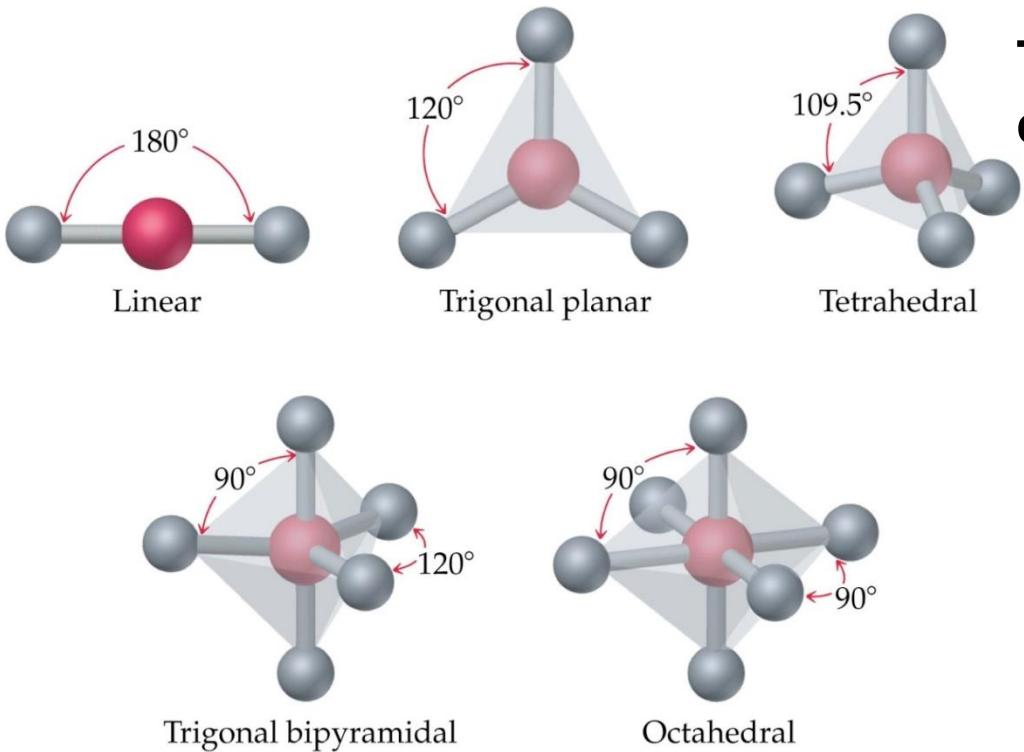
Each C is sp hybridized and has two unhybridized p orbitals.



Predicting the Shapes of Molecules: VSEPR Theory

Valence Shell Electron Pair Repulsion Theory

- In order to limit electrostatic repulsion, electron pairs in the orbitals around the central atom stay as far apart as possible

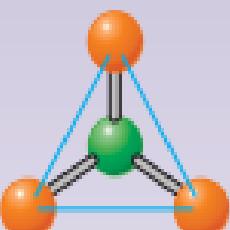
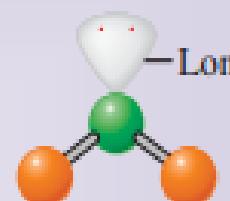


The *number of electron pairs* around the central atom determine *molecular geometry*....

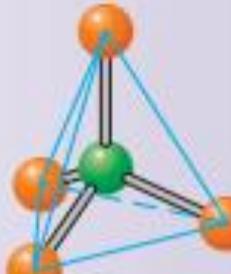
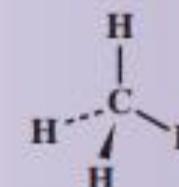
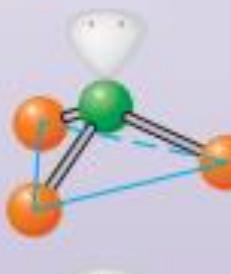
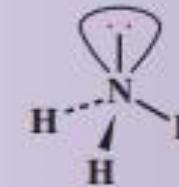
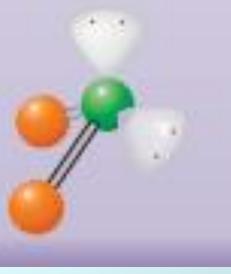
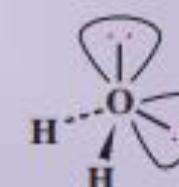
- ✓ 2 bonding pairs → linear (Bond angle = 180°)
- ✓ 3 bonding pairs → planar triangle (Bond angle = 120°)
- ✓ 4 bonding pairs → tetrahedral (Bond angle = 109.5°)
- ✓ 5 bonding pairs → trigonal bipyramidal
(Bond angles = 90° and 120°)
- ✓ 6 bonding pairs → octahedral (Bond angle = 90°)

Five basic molecular shapes

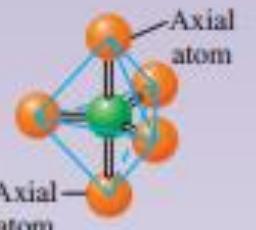
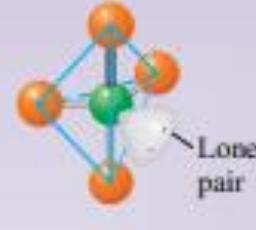
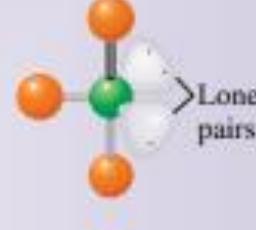
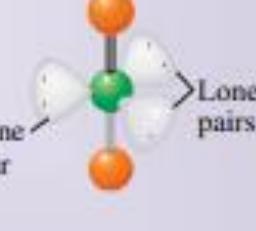
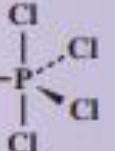
Predicting the Shapes of Molecules: VSEPR Theory

Electron Pairs			Arrangement of Pairs	Molecular Geometry	Example
Total	Bonding	Lone			
2	2	0	Linear	AX_2 	BeF_2 $\text{F}—\text{Be}—\text{F}$
3	{ 3 2 }	{ 0 1 }	Trigonal planar Bent (or angular) AX_2	AX_3  AX_2 	BF_3 $\begin{array}{c} \text{F} \\ \\ \text{B} \\ / \backslash \\ \text{F} \end{array}$ SO_2 

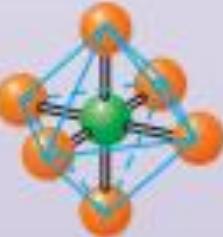
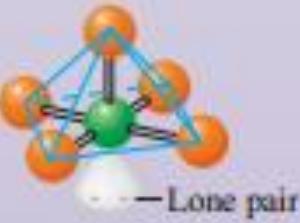
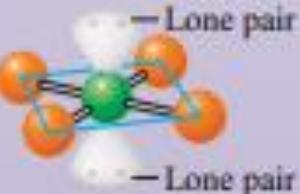
Predicting the Shapes of Molecules: VSEPR Theory

Electron Pairs			Arrangement of Pairs	Molecular Geometry	Example
Total	Bonding	Lone			
4	4	0	Tetrahedral		CH_4 
	3	1			NH_3 
	2	2			H_2O 

Predicting the Shapes of Molecules: VSEPR Theory

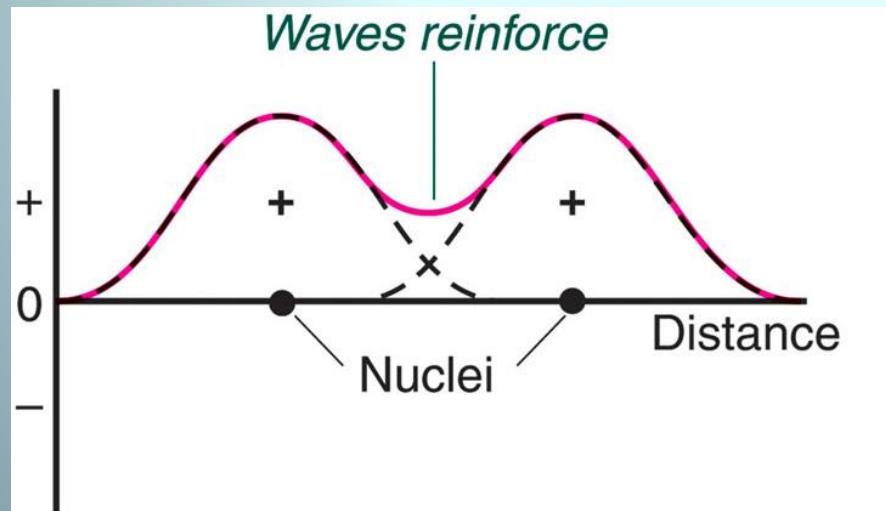
Electron Pairs			Arrangement of Pairs	Molecular Geometry	Example
Total	Bonding	Lone			
5	5	0		Trigonal bipyramidal AX_5	 Axial atom Axial atom
	4	1		Seesaw (or distorted tetrahedron) AX_4	
	3	2	Trigonal bipyramidal	T-shaped AX_3	
	2	3		Linear AX_2	
					PCl_5 
					SF_4 
					ClF_3 
					XeF_2 

Predicting the Shapes of Molecules: VSEPR Theory

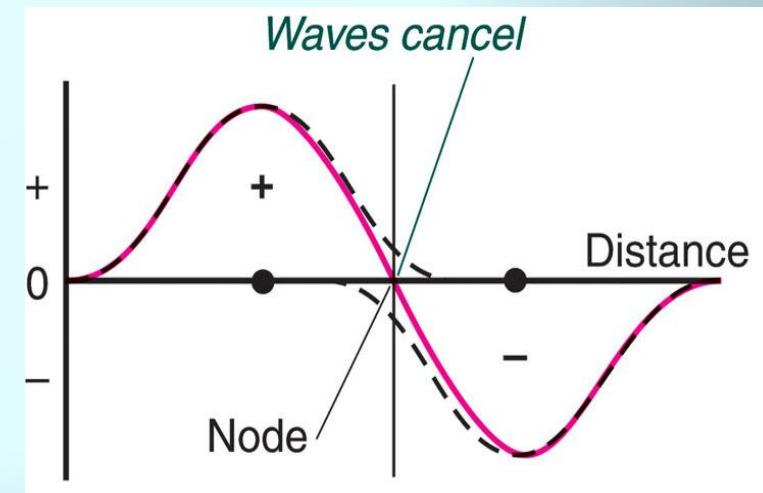
Electron Pairs Total Bonding Lone	Arrangement of Pairs	Molecular Geometry	Example
$\left.\begin{array}{ccc} 6 & & 0 \\ 6 & 5 & 1 \\ 4 & & 2 \end{array}\right\}$	Octahedral	<p>Octahedral AX_6</p>  <p>Square pyramidal AX_5</p>  <p>Square planar AX_4</p> 	SF_6 
			IF_5 
			XeF_4 

2. Molecular Orbital (MO) Theory

- The combination of orbitals to form bonds is viewed as the combination of *wave functions*. *Atomic* wave functions (AOs) combine to form *molecular* wave functions (MOs).
- Addition* of AOs forms a *bonding MO*, which has a region of *high* electron density between the nuclei.
- Subtraction* of AOs forms an *antibonding MO*, which has a *node*, or region of zero electron density, between the nuclei.



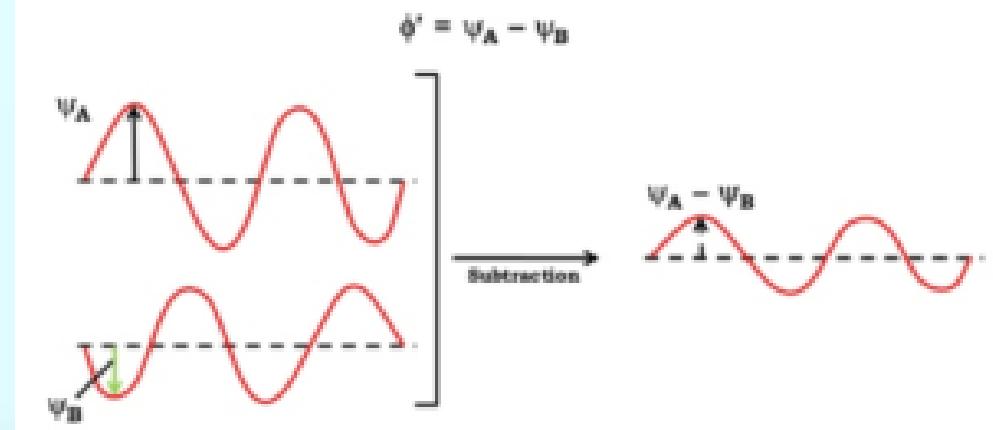
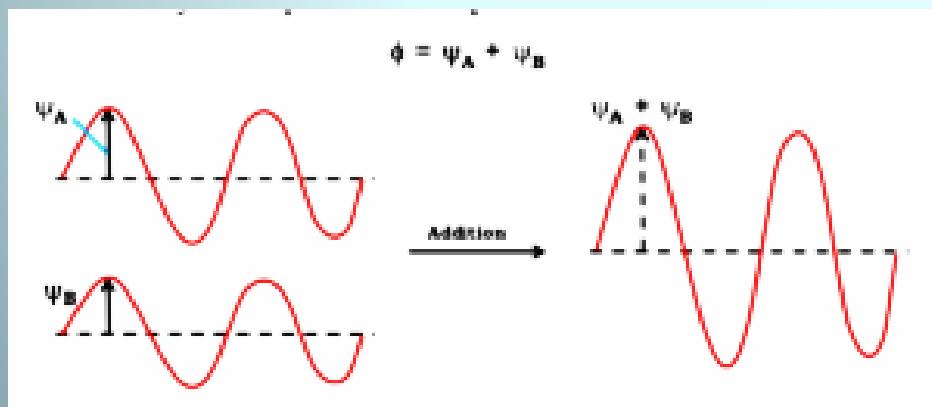
Amplitudes of wave functions added



Amplitudes of wave functions subtracted

Formation of Molecular Orbitals

- An atomic orbital is an electron wave; the waves of the two atomic orbitals may be in phase or out of phase. Suppose Ψ_A and Ψ_B represent the amplitude of the electron wave of the atomic orbitals of the two atoms A and B.
- Case 1 – Bonding MO: When the two waves are in phase so that they add up and amplitude of the wave is $\Phi = \Psi_A + \Psi_B$
- Case 2 – Antibonding MO: when the two waves are out of phase, the waves are subtracted from each other so that the amplitude of the new wave is $\Phi' = \Psi_A - \Psi_B$



Characteristics of Bonding Molecular Orbitals

- The probability of finding the electron in the internuclear region of the bonding molecular orbital is greater than that of combining atomic orbitals.
- The electrons present in the bonding molecular orbital result in the attraction between the two atoms.
- The bonding molecular orbital has lower energy as a result of attraction and hence has greater stability than that of the combining atomic orbitals.
- They are formed by the additive effect of the atomic orbitals so that the amplitude of the new wave is given by $\Phi = \Psi_A + \Psi_B$
- They are represented by σ , π , and δ

Characteristics of Anti-bonding Molecular Orbitals

- The probability of finding the electron in the internuclear region decreases in the anti-bonding molecular orbitals.
- The electrons present in the anti-bonding molecular orbital result in the repulsion between the two atoms.
- The anti-bonding molecular orbitals have higher energy because of the repulsive forces and lower stability.
- They are formed by the subtractive effect of the atomic orbitals. The amplitude of the new wave is given by $\Phi' = \Psi_A - \Psi_B$
- They are represented by σ^* , π^* , δ^*

Why are Antibonding Orbitals Higher in Energy?

- The energy levels of bonding molecular orbitals are always lower than those of anti-bonding molecular orbitals.
- This is because the electrons in the orbital are attracted by the nuclei in the case of bonding Molecular Orbitals whereas the nuclei repel each other in the case of the anti-bonding Molecular Orbitals.

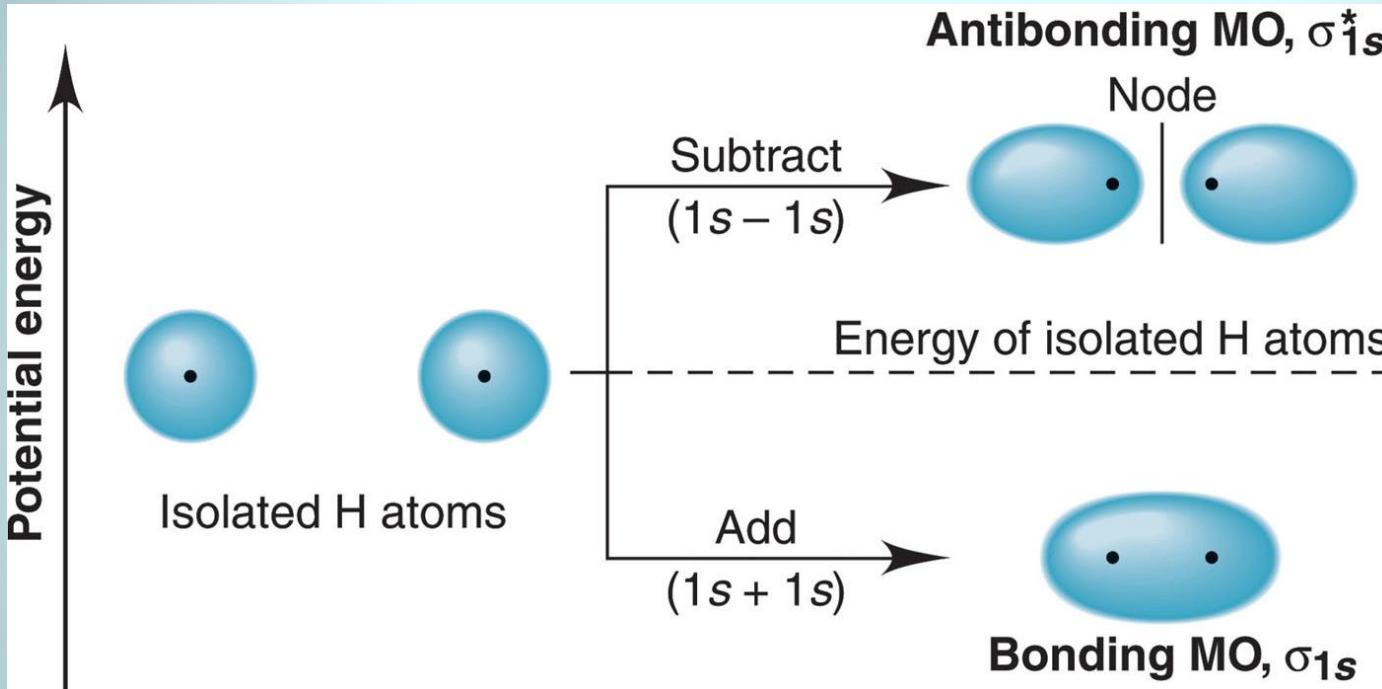
According to the Molecular Orbital Theory, the filling of orbitals takes place according to the following rules:

- **Aufbau's principle:** Molecular orbitals are filled in the increasing order of energy levels.
- **Pauli's exclusion principle:** In an atom or a molecule, no two electrons can have the same set of four quantum numbers.
- **Hund's rule of maximum multiplicity:** Pairing of electrons doesn't take place until all the atomic or molecular orbitals are singly occupied.

2. Molecular Orbital (MO) Theory

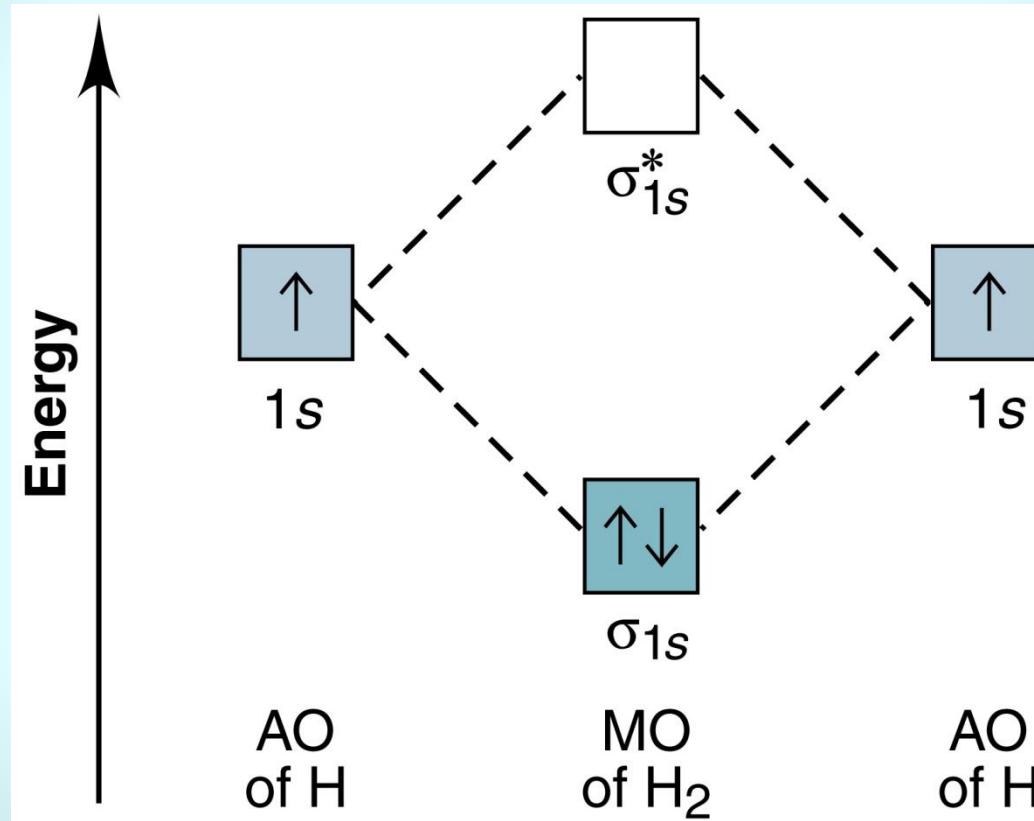
- A *MO diagram*, just like an atomic orbital diagram, shows the relative energy and number of electrons in each MO.
- The MO diagram also shows the AOs from which each MO is formed.
- Bond order is calculated as follows:
$$\frac{1}{2}[(\text{no. of } e^- \text{ in bonding MO}) - (\text{no. of } e^- \text{ in antibonding MO})]$$

Contours and energies of bonding and antibonding MOs of H₂



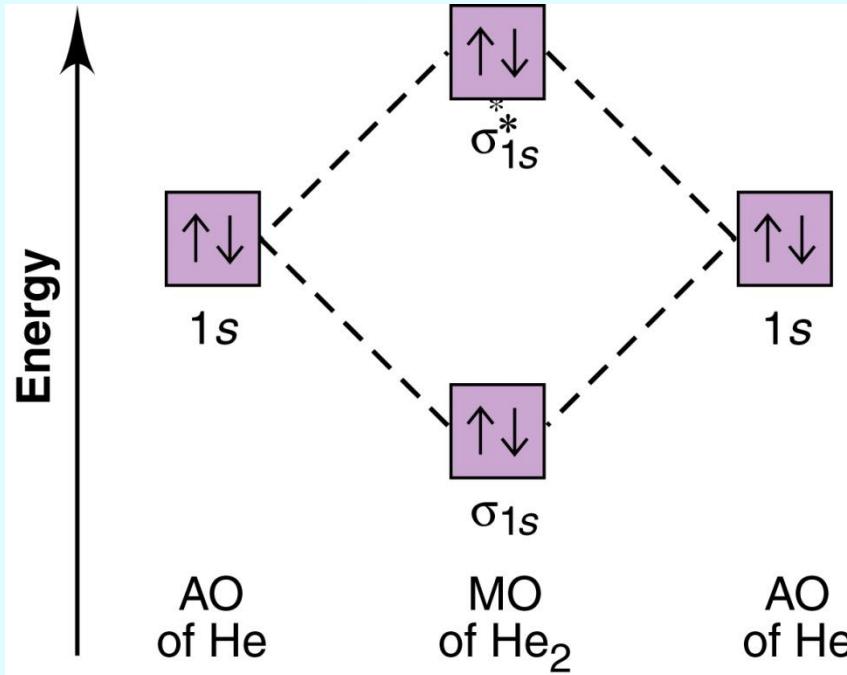
The bonding MO is lower in energy and the antibonding MO is higher in energy than the AOs that combined to form them.

Molecular orbital diagram of H₂ molecule



$$\text{H}_2 \text{ bond order} = \frac{1}{2} (2 - 0) = 1$$

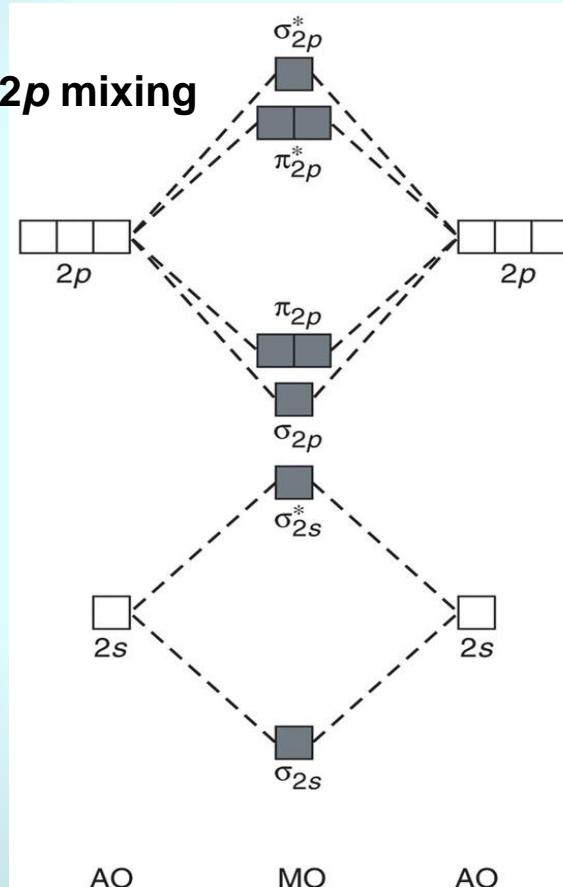
Molecular orbital diagram of He_2 molecule



He_2 bond order = 0

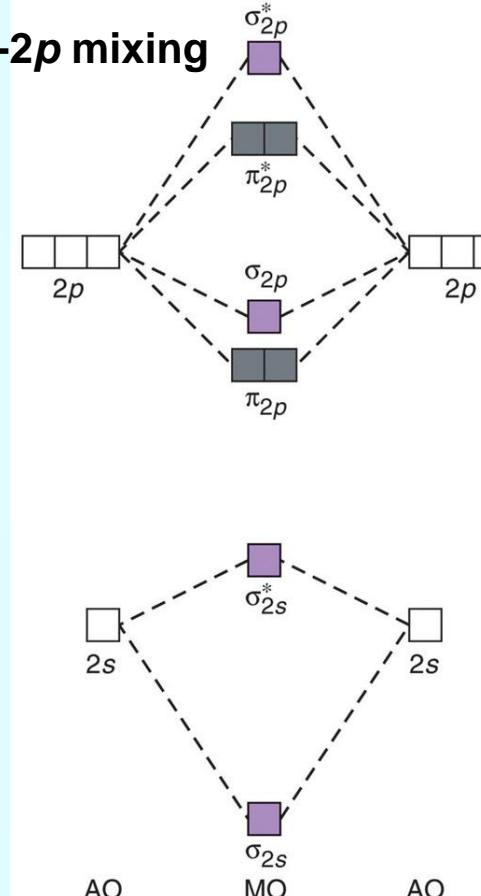
Relative MO energy levels for homonuclear diatomic molecules

without 2s-2p mixing



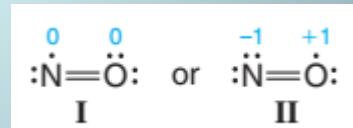
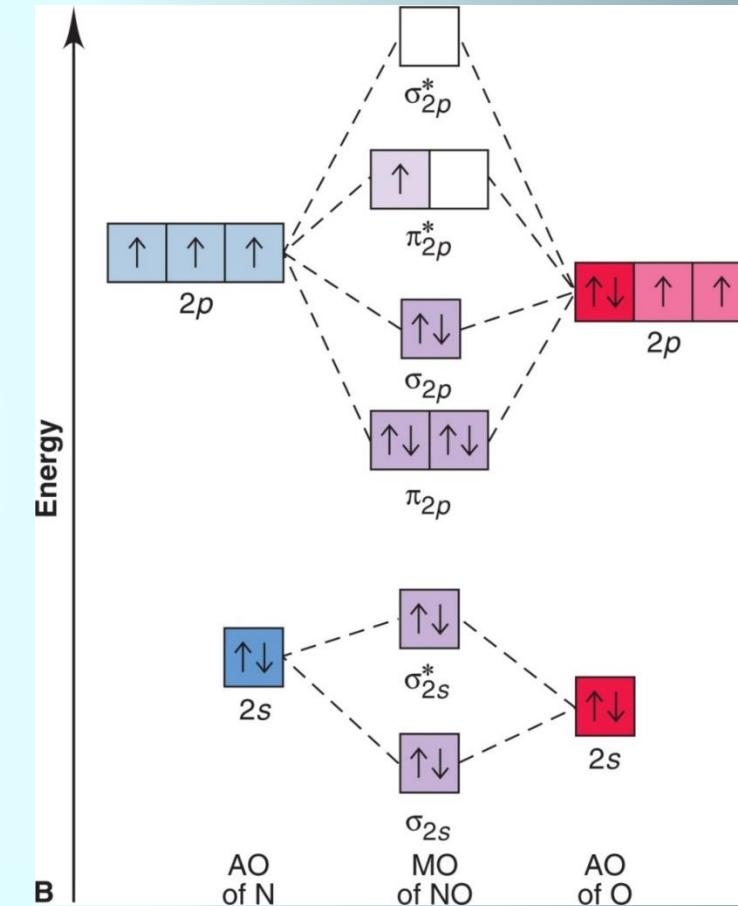
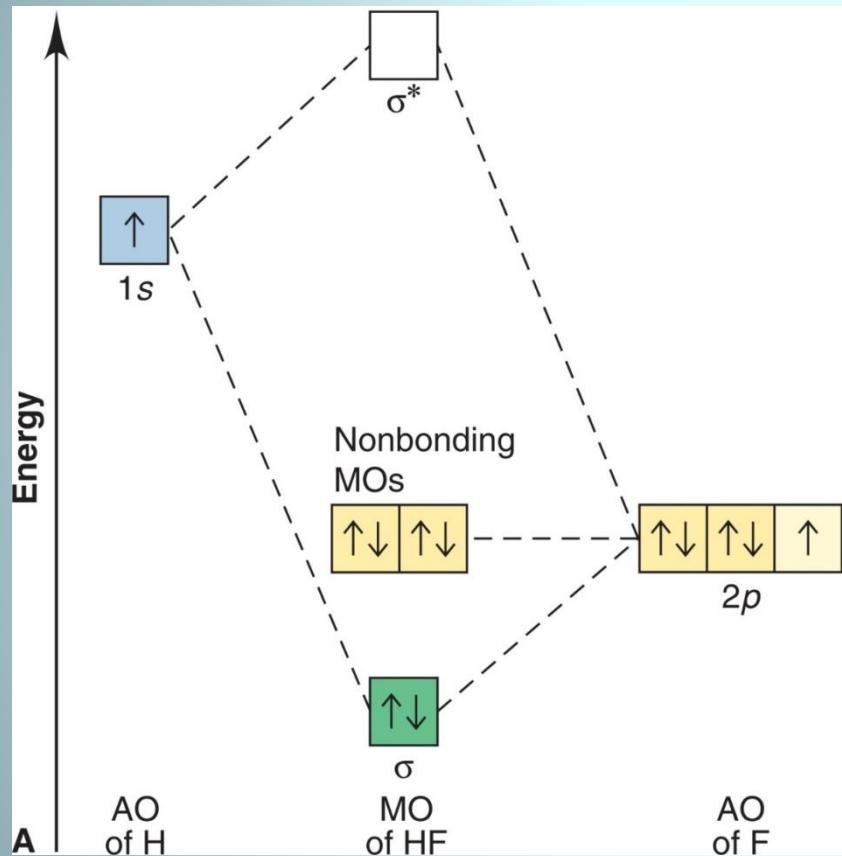
MO energy levels for
 O_2 , F_2 , and Ne_2

with 2s-2p mixing



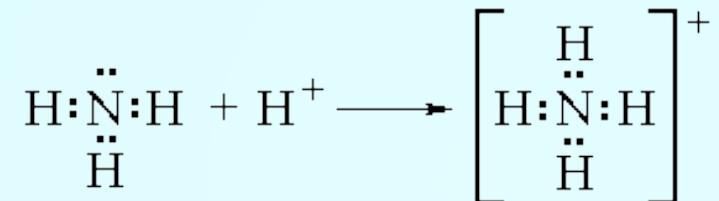
MO energy levels
for B_2 , C_2 and N_2

The MO diagram for HF and NO



Coordinate Covalent Bonding

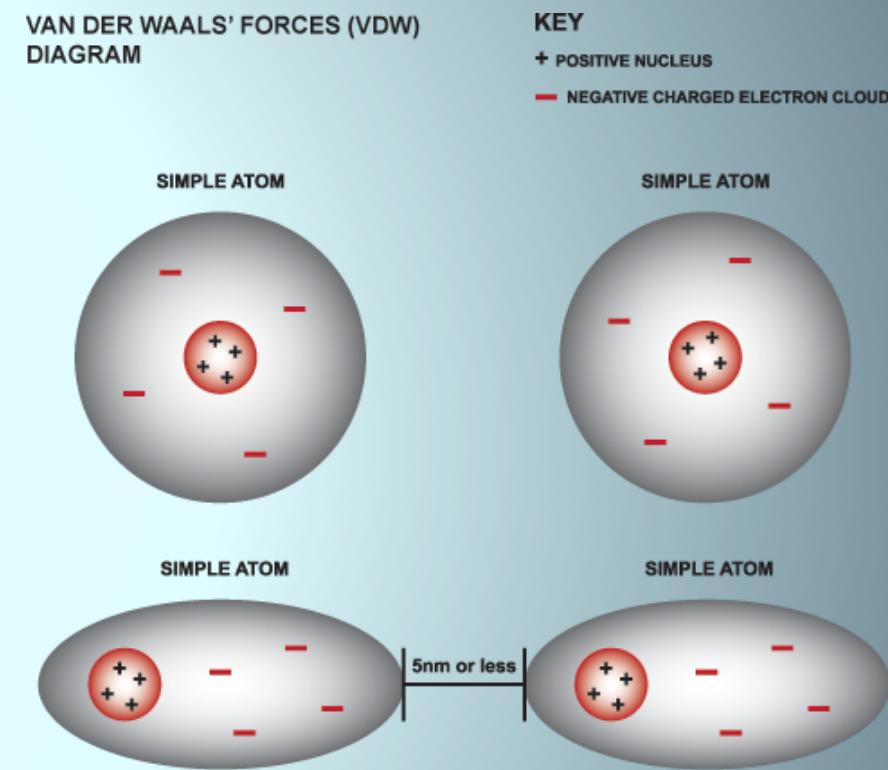
A coordinate bond (also called a dative covalent bond) is a covalent bond (a shared pair of electrons) in which both electrons come from the same atom.



- Atom that shares an electron pair from itself is termed as the donor.
- The other atom which accepts these shared pair of electrons is known as a receptor or acceptor.
- The bond is represented with an arrow \rightarrow , pointing towards acceptor from the donor atom.
- After sharing of electron pair each atom gets stability.

Van der Waals Attraction Force

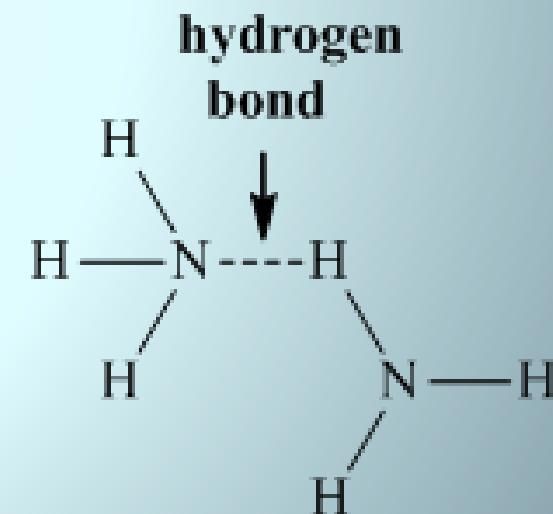
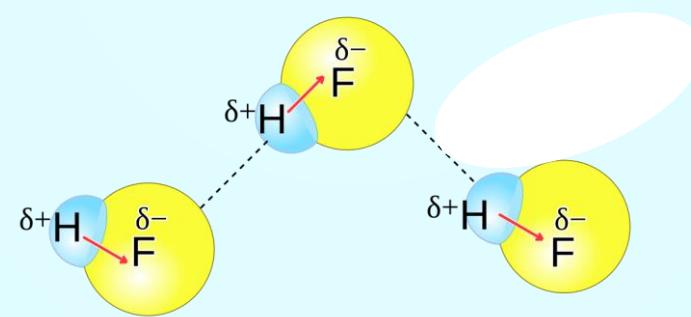
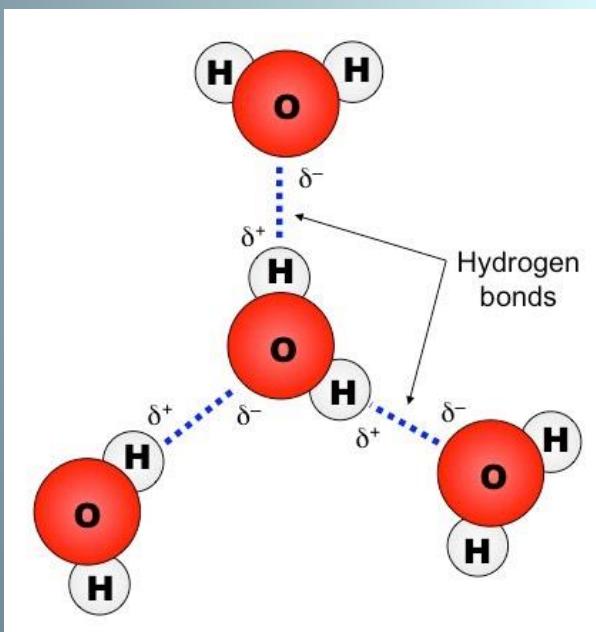
- Van der Waals forces are weak intermolecular forces that are dependent on the distance between atoms or molecules.
 - These forces arise from the interactions between uncharged atoms/molecules.
 - These forces are significantly weaker than ionic and covalent bonds.
 - Van der Waals forces are short-range forces. Their magnitude is high when the atoms/molecules in question are close to each other.
 - No directional characteristic can be attributed to these forces.
 - Increases with molecular mass.



When two atoms come within 5 nanometers of each other, there will be a slight interaction between them, thus causing polarity and a slight attraction.

Hydrogen Bonding

- A special class of intermolecular attraction force that arise due to the dipole-dipole interaction between a hydrogen atom that is bonded to a highly electronegative atom and another highly electronegative atom while lies in the vicinity of the hydrogen atom.



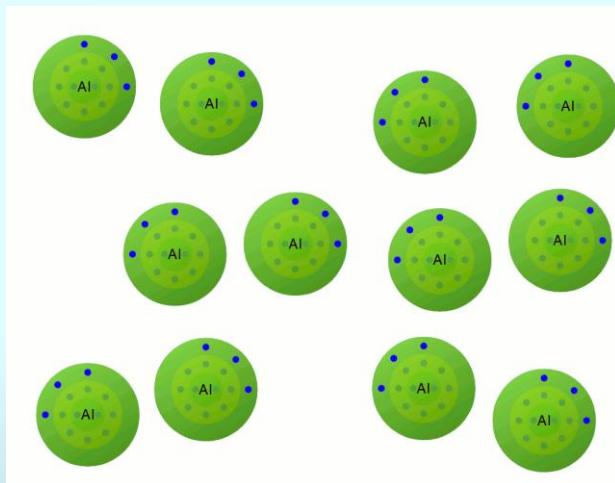
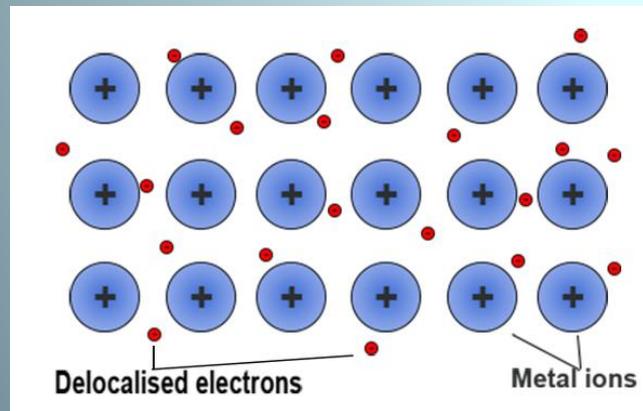
Hydrogen Bonding

Features of Hydrogen bonding

- The molecule must contain a highly electronegative atom linked to hydrogen atom.
- The size of the electronegative atom should be small.
- Only F, O and N are capable of forming hydrogen bonding.
- Molecules having hydrogen bonding have high melting and boiling points. Example: H_2O , H_2S ; NH_3 , PH_3
- Density of ice is lower than water due to cage-like structure of water in solid ice.

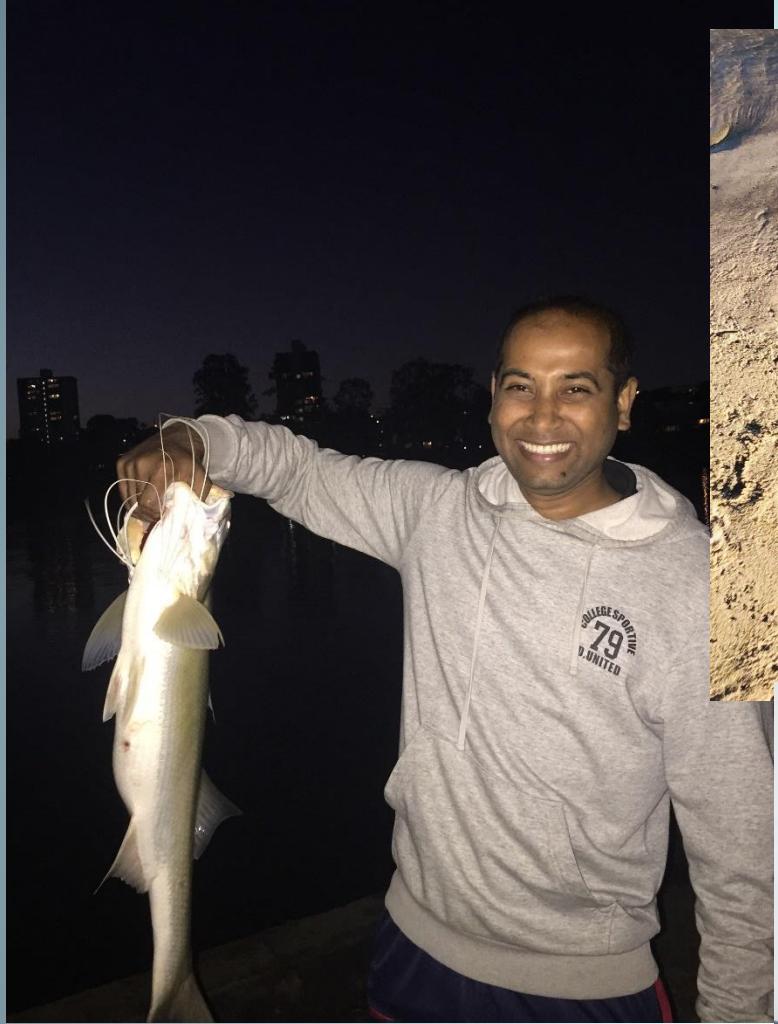
Metallic Bonding

- Is the force, that holds atoms together in a metallic substance.
- The outermost electron shell of each of the metal atoms overlaps with a large number of neighbouring atoms.
- As a consequence, the valence electrons continually move from one atom to another, and not associated with any specific pair of atoms.
- In short, unlike covalently bonded substances, the valence electrons are not localized, and capable of wandering relatively freely throughout the entire crystal.



The strength depends on –

- Total number of delocalized electrons
- Ionic radius of the cation

























Energy-Smart Villages | Team Krishi Bondhu

Mentor: Dr. Md. Mahbub Alam, Assistant Professor, BUET

Team: Farsia Kawsar Chowdhury | Shorup Chanda | Emon Roy Bappy | Mohammad Tamimur



Photo: © GIZ/ Shorup Chanda

Crop preservation facilities are inadequate compared to our farmers' needs in south Asian countries like Bangladesh. They are not getting even half of the price if they sell it after harvesting than they would have sold it after storage a few days after production and processing. As 85% of the vegetables and dairy products are perishable. The tendency of rural farmers is to sell the produced products at the same day they harvest. In some cases, they do not even harvest. Those are just rotting on the field and they don't get any price for that. Not having stable electricity is hindering them from accessing preservation facilities in those areas. This group includes small marginal farmers and vegetable vendors, dairy product vendors and people associated with medicine storage. Team Krishi Bondhu aims to reduce post-harvest losses and help the rural farmers to boost their income. Not only that, our project can bring a significant decrease in carbon footprint. Our project STAR is for lower-income regions, where electricity is scarce and discontinuous for a long time. Our solar thermal adsorption refrigeration (STAR) technology can be an alternative to conventional refrigeration systems in these areas and other sites where there is a lack of reliable electric grid. It is a refrigeration technique that doesn't require electricity and can perform as a green solution of the current refrigeration techniques. We will be developing community based cold storages and single unit refrigerators using our technique so that rural villagers can preserve their vegetables, dairy products and medicines. By using our setup they will be able to double their everyday income by selling preserved products keeping it fresh. Not only income, this project also focuses on controlling urban migration and reducing pressure on the regular goods transports.

Thank You