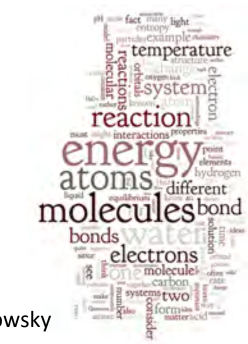
Yet More Bonding



Chemistry, Life, the Universe & Everything – Cooper & Klymkowsky

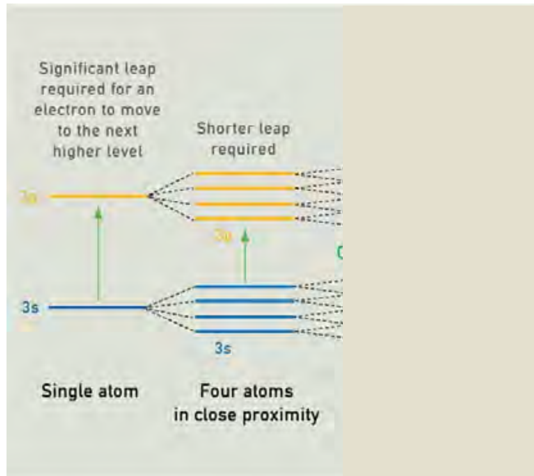
Metals

- Shiny
- Conduct electricity
- Malleable
- May be colored (gold, copper, etc) – silver is colorless
- How does bonding in metals explain their properties?

Bonding in metals

•Atomic orbitals (lots of them) combine with each other to form molecular orbitals (an equal number)

•As the number of MOs increases, the energy distance between them decreases.



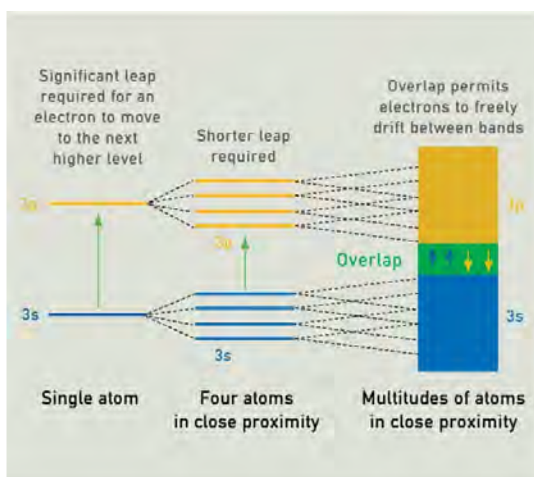
Bonding in metals

•Atomic orbitals (lots of them) combine with each other to form molecular orbitals (an equal number)

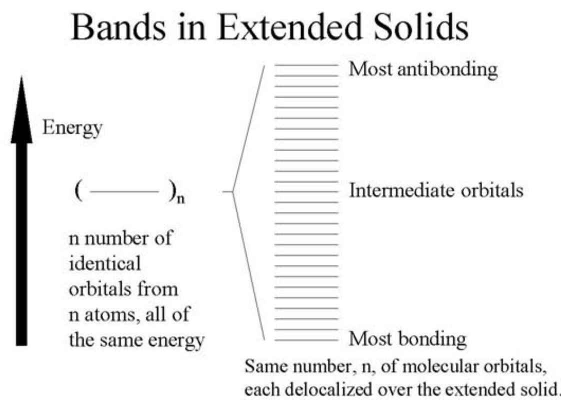
•As the number of MOs increases, the energy distance between them decreases.

•Forming bands of MOs – of almost continuous energy

•Electrons can move freely between MOs.



Extended MO's



Properties of metals

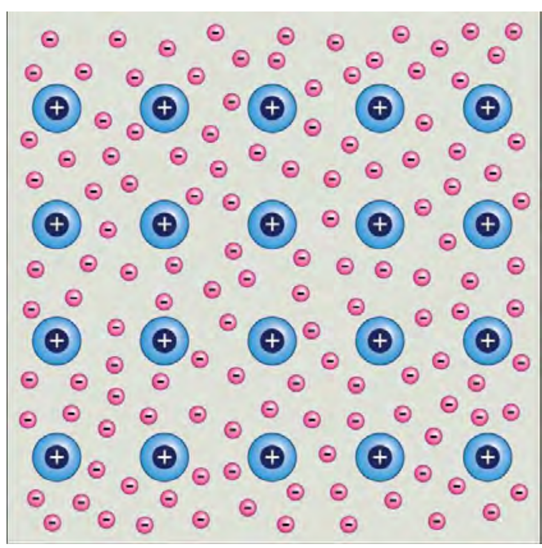
Because electrons can move freely around, metals conduct electricity

Because atoms can move with respect to one another, metals are malleable.

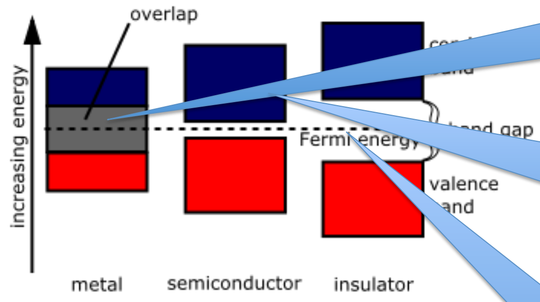
-Absorption of a photon will promote an electron to a higher energy level.

It immediately falls back down – emitting a photon – the metal shines (but not in the dark – why not?)

-The metal interacts with light of many wavelengths, so the metal appears white or colorless (silvery).



Band Theory



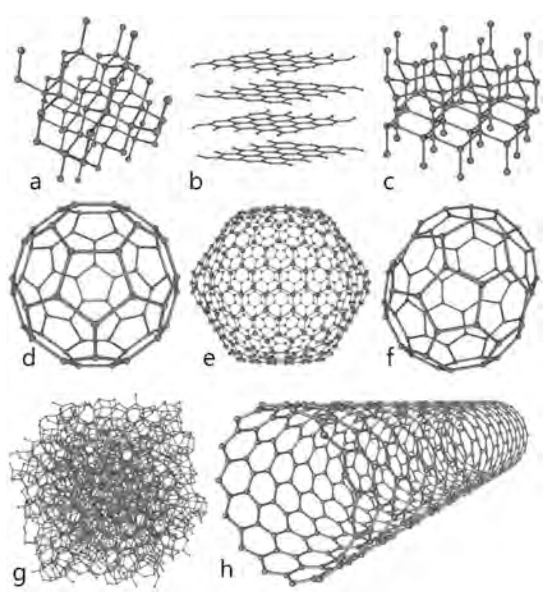
In metals the valence band (bonding MO's) overlaps with the conduction band (antibonding MO's)

In semi-conductors (eg Si, Ge) there is a small gap between the bands, these materials are often used for solar cells, and in computer equipment

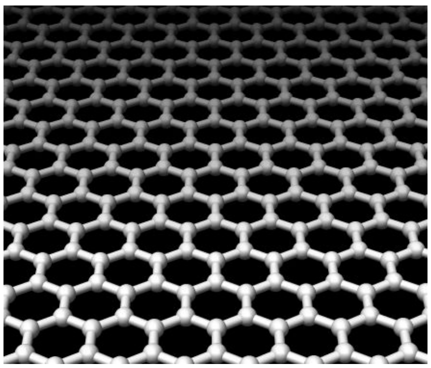
Materials that are insulators (eg diamond) there is a large energy gap between the valence and conduction band.

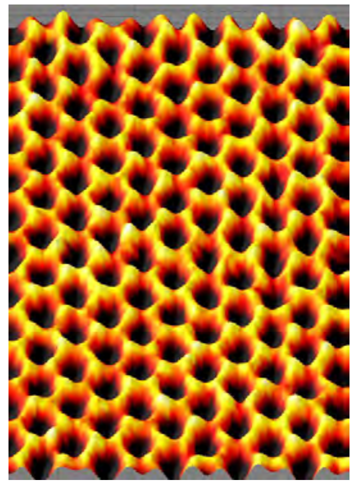
Allotropes of Carbon

a. Diamond
b. Graphite
c. Lonsdaleite (not common)
d. Buckminsterfullerene (C_{60})
e. C_{540}
f. C_{70}
g. Amorphous (soot)
h. Carbon (nanotube)

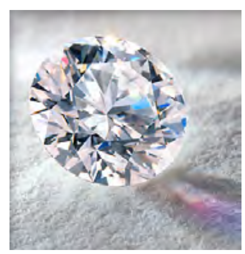


Graphene – one atom thick sheet (Nobel Prize 2010)





Diamonds



- Sparkly, translucent
- Hard
- High “melting” and “boiling” points
- Why?

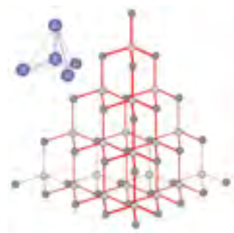
Bonding in Diamond

Each carbon forms 4 bonds to 4 identical carbons.

The bonds arrange themselves towards the corners of a 4 sided figure (a tetrahedron)

We call this geometry **tetrahedral**

The C-C-C bond angle is ~109°



If you wanted to "melt" diamond (tetrahedral carbon) what would have to happen? (draw a picture)

Why do metals melt and diamonds do not?

How come carbon forms 4 identical bonds in diamond?

- [He] $2s^2$ $2p^2$
- 4 valence electrons in atom – in different types of orbitals
- Should give different types of bonds, but the evidence indicates that **all four bonds are identical**

Models of Bonding

Molecular Orbital

- Atomic orbitals combine to form an equal number of molecular orbitals
- Each orbital can contain up to two electrons
- Electrons in bonding orbitals stabilize the system
- Electrons in anti-bonding orbital make it less stable

Valence Bond

- Atomic Orbitals overlap to form a bond
- Each bond made up of two electrons
- How to explain the idea that C forms 4 identical bonds in diamond?
  - **Hybridized orbitals**

Bonding in diamond (Valence Bond Model)

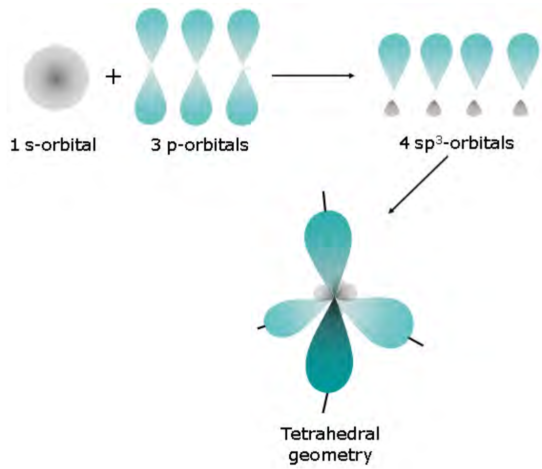
Atomic orbitals "hybridize" (mix up) to form bonding orbitals that then combine with orbitals from other atom to form a bond

To form 4 bonds – carbon hybridizes the 4 orbitals that are used for bonding.

They naturally assume a tetrahedral geometry (why?)

Since one s and three p orbitals combine, we call them sp^3 orbitals

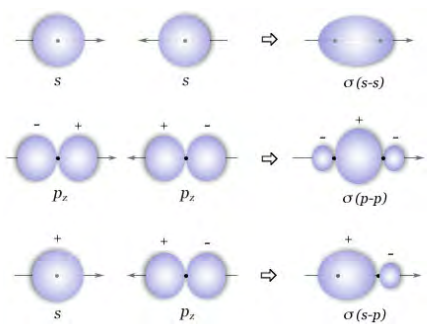
When the hybrid orbitals combine there is a large gap between the bonding and antibonding molecular orbitals

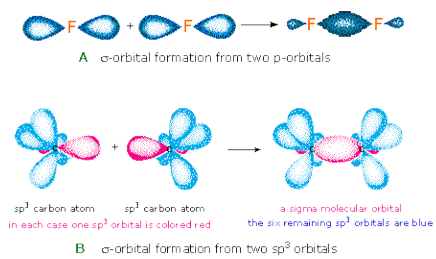


Bonding in tetrahedral C

- Hybridized atomic orbitals (sp^3) give rise to strong directed bonds.
  - Giving rise to high mp/decomposition temperature – because these bonds have to be broken to melt diamond (in fact diamond decomposes rather than "melts")
- These bonds are "sigma bonds"

Sigma bonds





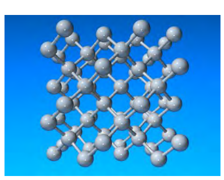
Comparison of diamond and graphite

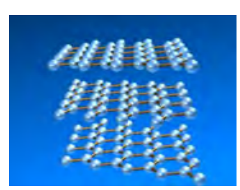
Diamond

- High mp
- Hard
- Brittle (breaks along planes)
- Translucent (lets light through)
- Does not conduct electricity

Graphite

- High mp
- Soft
- Slippery
- Grey, shiny
- Conducts electricity

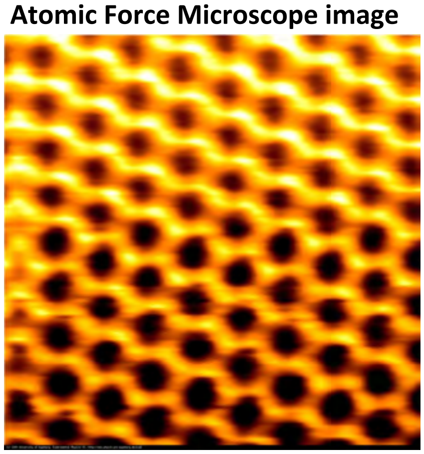




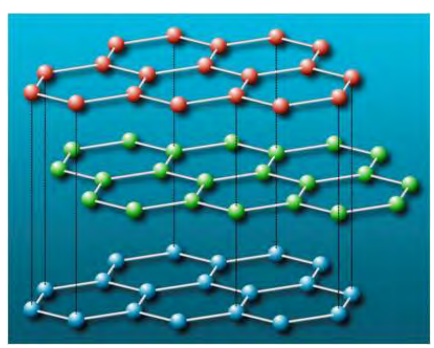
Diamond and graphite are made out of carbon atoms only – how can they have such different properties?

Graphite

Atomic Force Microscope image



Molecular model showing sheets



Bonding in graphite

One s and two p orbitals hybridize to give three sp^2 orbitals

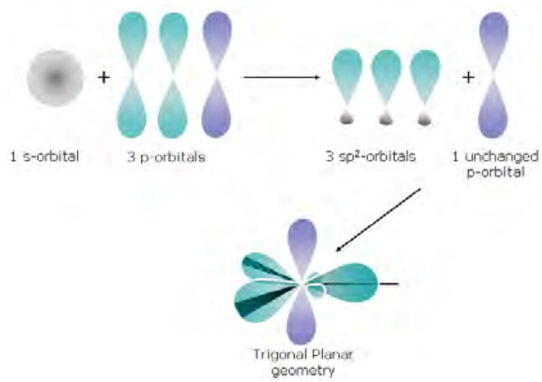
Geometry is called trigonal planar

C-C-C bond angle is 120

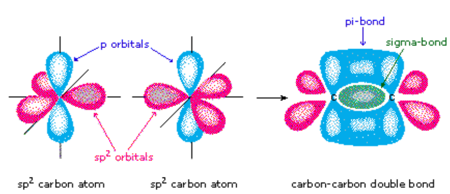
When the sp^2 hybrid orbitals combine they form **sigma** bonding molecular orbitals.

There is a p orbital left over.

These p orbitals (one on each carbon) combine side to side to form a large number of **Molecular Orbitals**

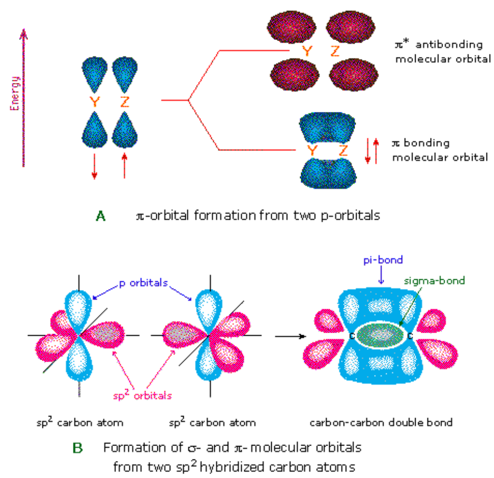


Sigma and pi bonds



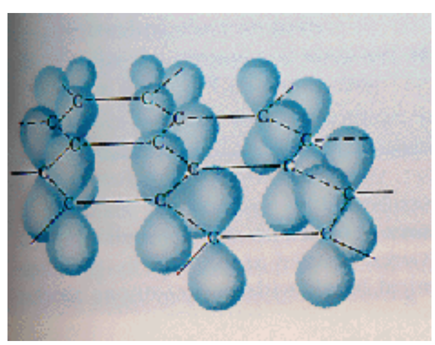
B Formation of σ- and π-molecular orbitals from two sp^2 hybridized carbon atoms

Sigma and pi bonds



Graphite

- Has a "localized" sigma bond framework (explained by overlap of hybridized orbitals)
- Has a "delocalized" pi network over the whole sheet of atoms (explained by delocalized pi molecular orbitals)



Graphite properties explained

- Slippery – sheets can slide over each other – only "held together" by LDF's
- Graphite conducts electricity because it has delocalized pi MOs over the whole structure
- Shiny – because it can absorb and emit photons (just like metals)