01D_Carbon

Carbon: Discover the origin of bonding in tetragonal diamond and hexagonal graphene

•Start with the electron orbits in single atoms of carbon

•Consider interaction between carbon atoms in terms of the hybridization of orbitals.

•Above results in two configurations known as sp^3 and sp^2, the first leads to tetragonal structure of diamond and the second to the hexagonal structure of graphene. Note the sp^3 implied four bonds (tetragonal) while sp^2 implies three.

Electron Orbitals in single carbon atom

The atomic weight of carbon is 12, i.e., it has six protons and six neutrons in the nucleus, and six electrons orbiting the nucleus.

The occupancy of electrons in successive orbitals is given by $2n^2$, where n=1, n=2, etc.

n=1 can contain 2 electronic

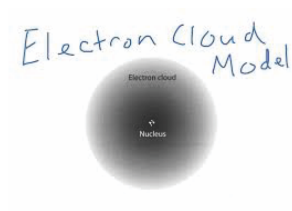
n=2 can contain 8 electrons

Therefore in carbon n=1 is filled while n=2 is half filled, i. e. it has four electrons.

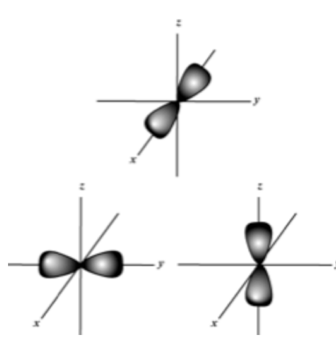
The shape of the electron clouds surrounding the nucleus

We shall consider only the "s" and the "p" orbitals.

-s orbitals are spherical in shape and can hold two electrons.



-p orbitals have two lobes, with three sets aligned along the three Cartesian axes as in



Each lobe can hold two electrons; therefore the p orbitals can hold a maximum of 6 electrons.

The orbitals in n=1, and n=2 are as follows n=1 has 1s orbital which can hold two electrons $1s^1$ and $1s^2$

n=2 has one 2s orbital which holds two electrons $2s^1$ and $2s^2$;

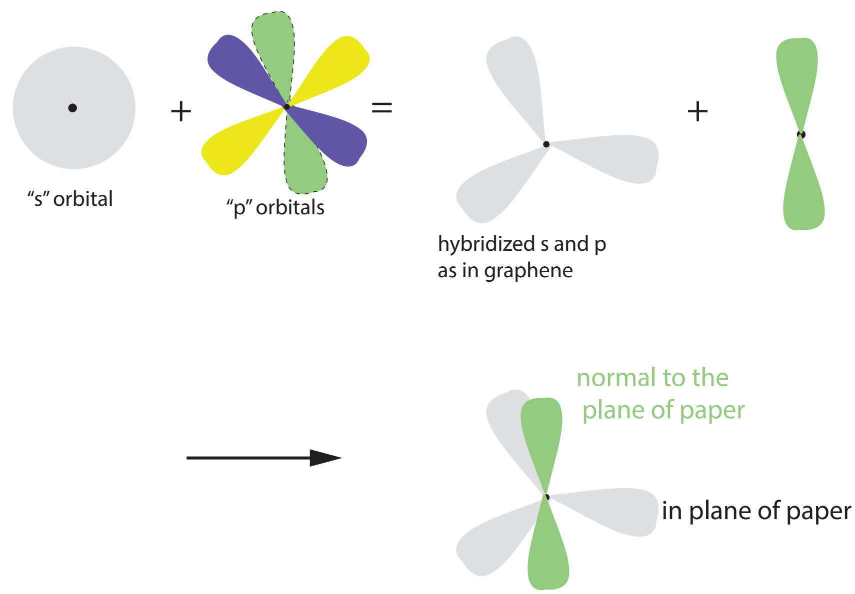
and three 2p orbitals, each having a capacity of 2 electrons, that is, six in total.

Therefor n=2 can hold a maximum of two 2s and six 2p electrons: eight in total.

Hybridization of s and p electron "lobes"

There are two types sp^2 and sp^3

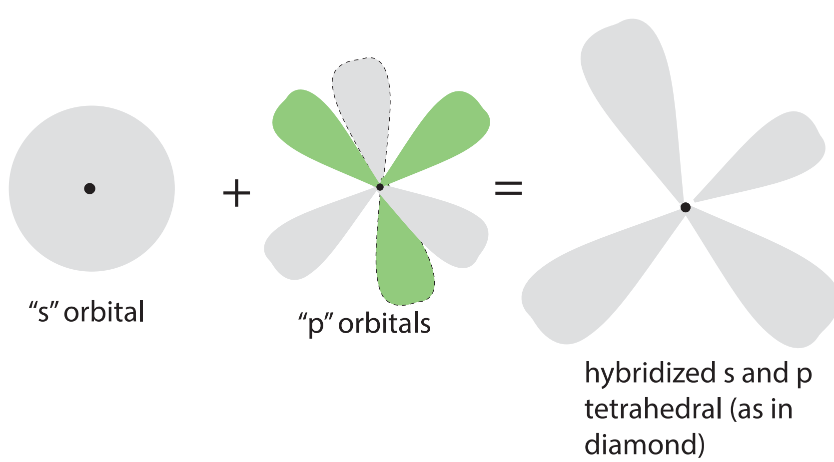
sp^2 hybridization



The total number of electrons that can be accommodated must remain constant in the hybridized configuration, that is a maximum of 8 electrons. However, carbon has only four electrons in the second shell. In the sp^2 hybridization these four electrons, three are distributed within the three lobes in the plane of the paper, while one electron resides in the "green" lobe perpendicular to the plane of the paper.

Note that graphite has a layered structure so that three electrons are shared with three neighboring carbon atoms in covalent bonding while the four is shared between the layers. Thus, the in-plane bonding is much stronger than the out of plane bonding.

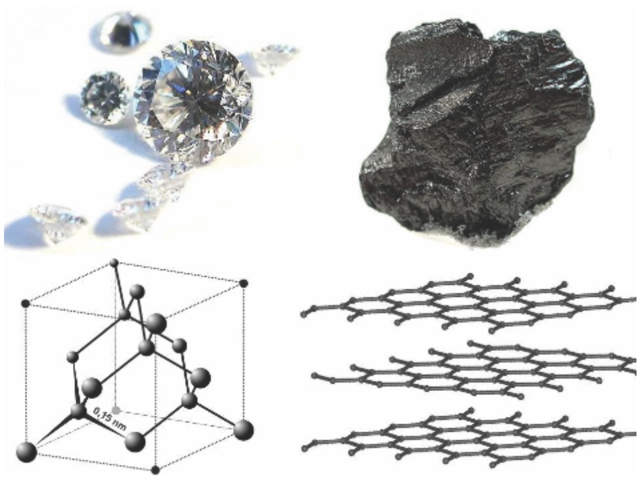
sp^3 hybridization



In sp^3 hybridization the three p orbitals and one s orbital combine to create four orbitals that are equally aligned with respect to the center as in tetrahedral configuration. Each of the four lobes may now hold 2 electrons, for a total of 8 electrons as required in n=2.

In carbon there are four electrons in n=2, therefore there is on average one electron per lobe. These electrons for covalent bonds with four nearest neighbors to find a full shell one half the time.

The Structure of Diamond and Graphite



Which is more stable (thermodynamically speaking)?

Actually the energy of formation of graphite is approximately 2 kJ/mol deeper than of diamond, that is, graphite is the more stable phase although just slightly. That is the reason that graphite is more commonly found in nature than is diamond.

Note

•Remember that hybridization does not change the total number of electrons that can be accommodated within on shell.

•For example, the one 2s and the three 2p orbitals can have a total of 8 electrons (2 in each). Similarly, the sp^2 hybridization creates three sp2 orbitals and one p orbital for a total of eight possible electrons.

•Similarly, sp^3 hybridization creates four orbitals with two electrons in each.

The Energy differences between States of the same elements