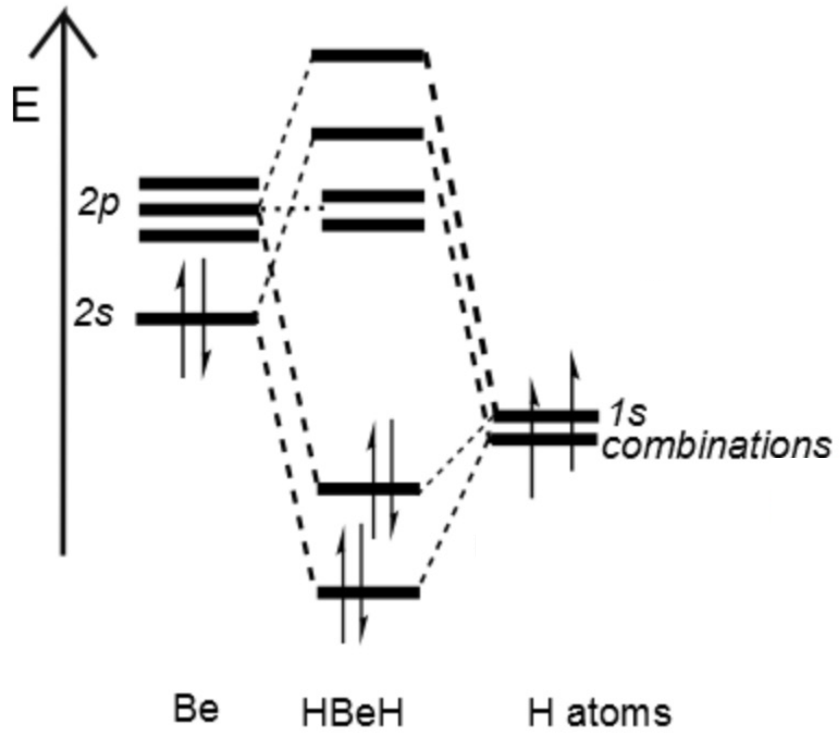
1. Hybrid molecular orbitals

A) Consider the methane molecule: CH_4

- What is its structure?
- Which hybrid orbitals and which bonds are formed?

B) Beryllium ($1s^2\ 2s^2$) and two hydrogen atoms form the linear BeH_2 molecule: HBeH.
The formation of the BeH_2 molecule is explained with the formation of two sp hybrid orbitals from the 2s orbital and one 2p orbital, for example the $2p_z$, if we choose z as interatomic axis. The resulting scheme for the molecular orbitals is shown in the figure.

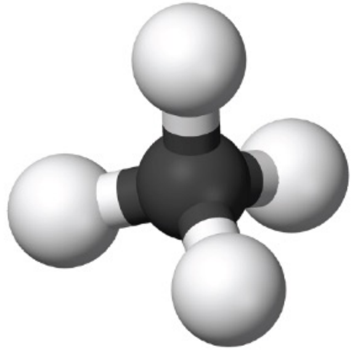
- Identify the levels of the sp and sp* orbitals in the scheme.
- Draw the corresponding molecular orbitals.



1. Solution - Hybrid molecular orbitals

A)

Methane has a tetrahedral structure, related to the formation of sp^3 hybrid orbitals.

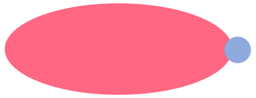


methane

Bonds: four σ bonds between the sp^3 and the four H 1s

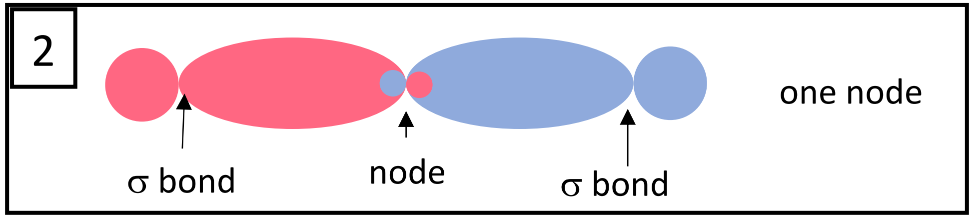
B)

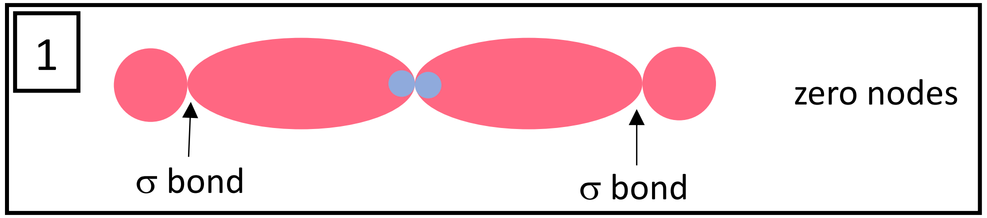
The sp orbitals form σ bonds with the H 1s orbitals.
Note the increasing number of nodes for increasing energy.
(When condensed, the BeH_2 molecules form polymers.)

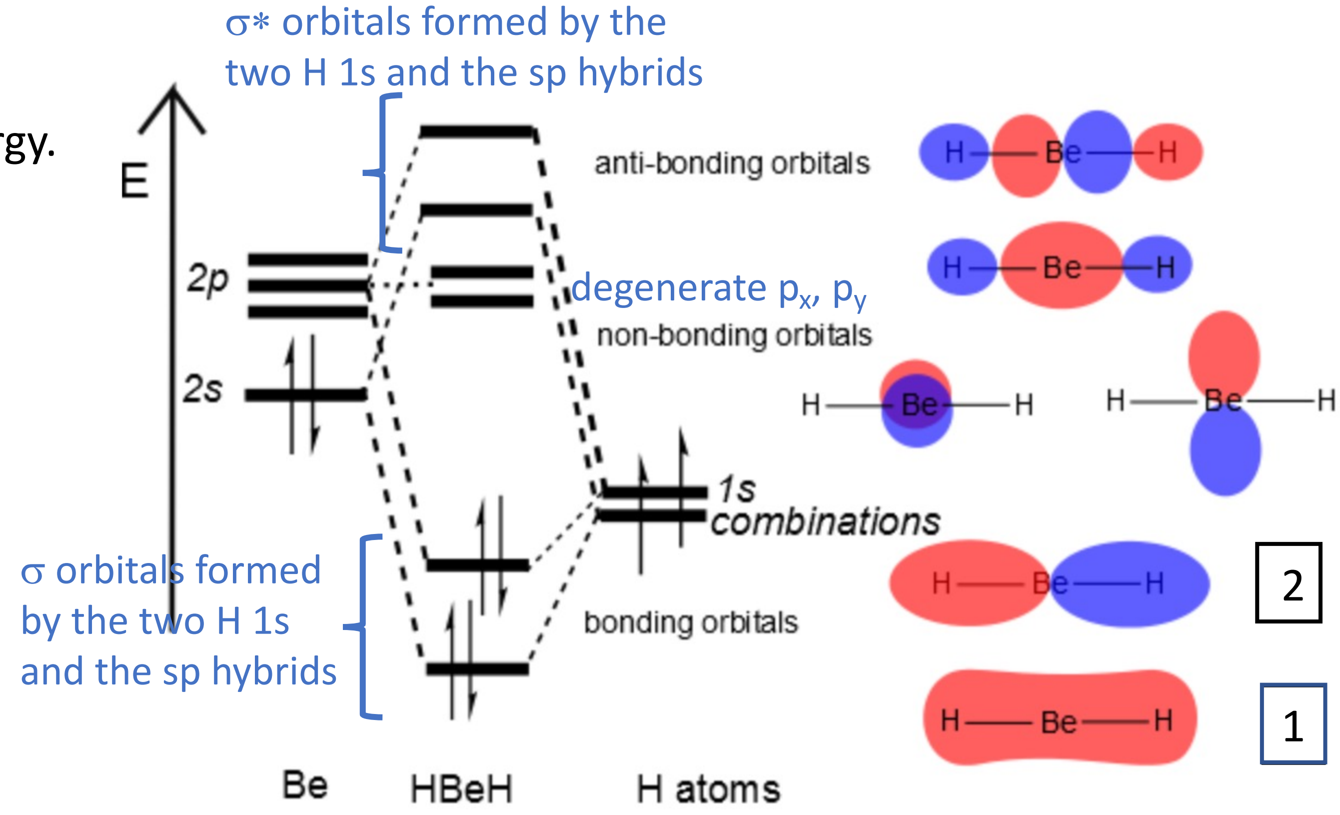


one sp orbital

H 1s orbital



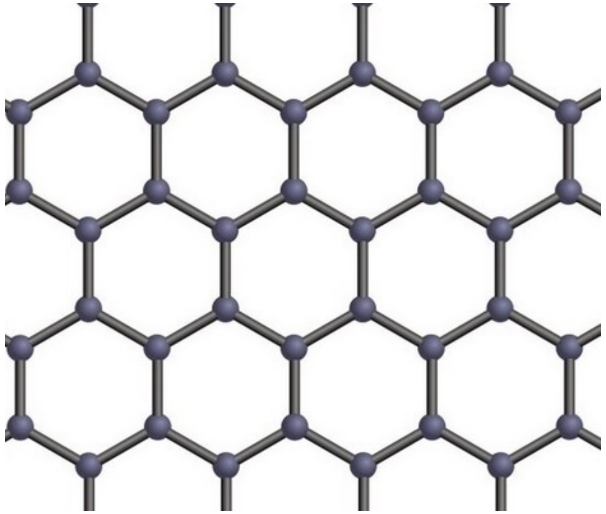




2. Graphene

Graphene is an allotrope of carbon consisting of a single layer of atoms arranged in a honeycomb structure.

- Which atomic orbitals participate into the bonding?
- What are the hybrid orbitals that are formed?
- Which types of bonds are formed and where?



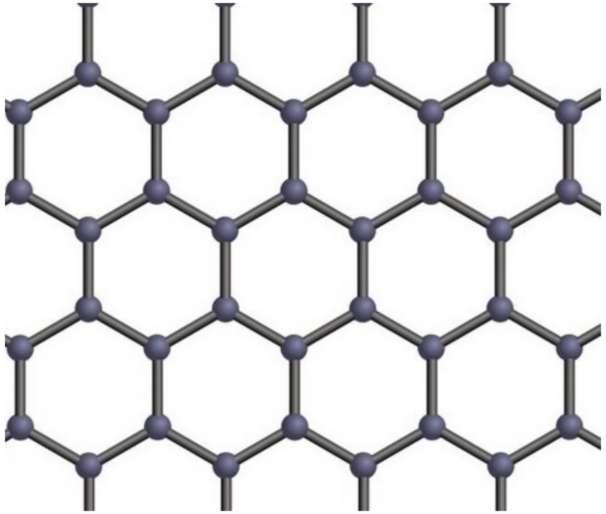
2. Solution - Graphene

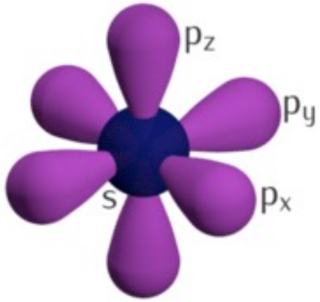
Carbon: $1s^2\ 2s^2\ 2p^2$

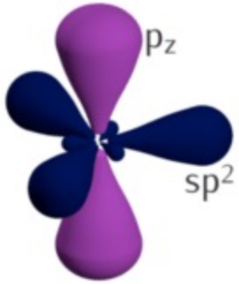
The orbitals 2s and 2p participate into the bonding

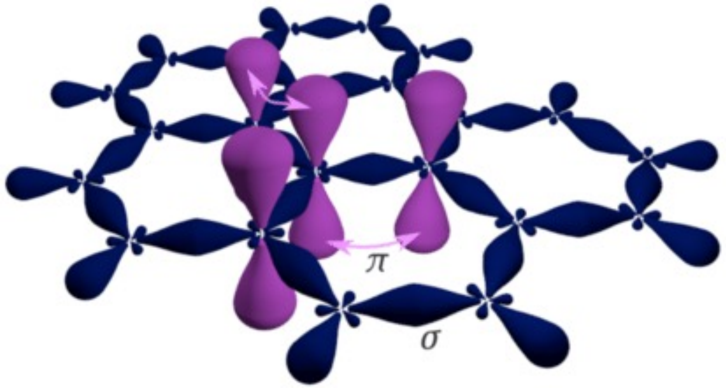
The planar structure is obtained thanks to the sp^2 hybridization

σ bonds between the sp^2 orbitals in the plane;
π bonds between the p_z orbitals perpendicular to the plane









Delocalized π orbitals