All orbital interaction diagrams have common features:

The number of atomic orbitals that combine is often called the basis set.

The number of orbitals in the basis set determines the number of new molecular orbitals that are created; for the H_2 molecule, two atomic 1s orbitals comprise the basis set and two new MOs are created.

Atomic orbitals can combine (overlap) in a constructive manner or destructive manner.

MOs that are higher in energy than the starting atomic orbitals are called antibonding MOs
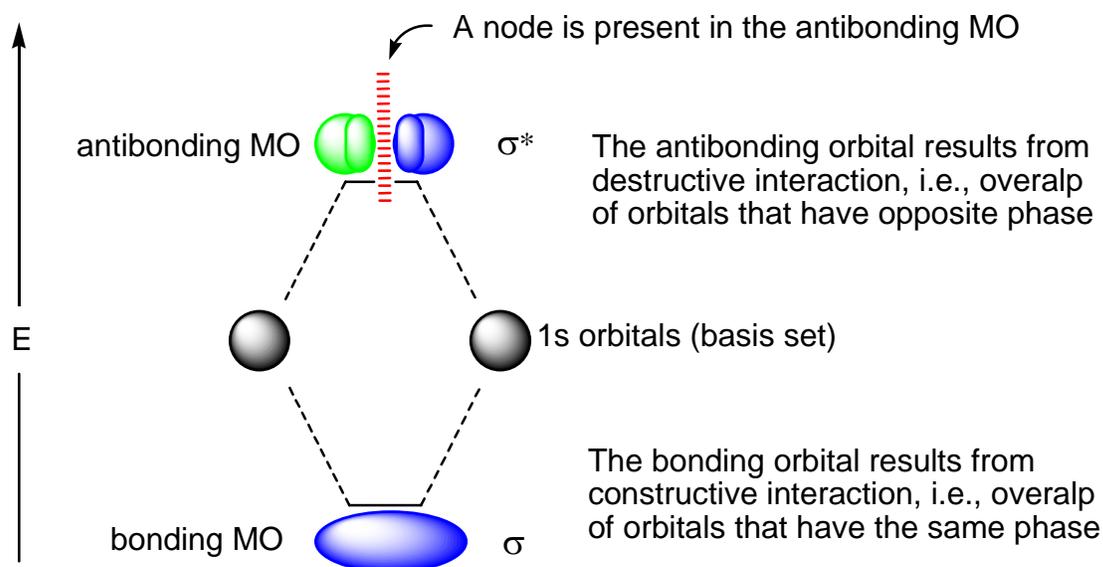
MOs that are lower in energy than the basis set are called bonding MOs

MO that are equal in energy to the starting atomic orbitals are labeled as non-bonding MOs (for example, the allyl system has non-bonding MOs)

Just like atomic orbitals, MO can hold zero, one or two electrons

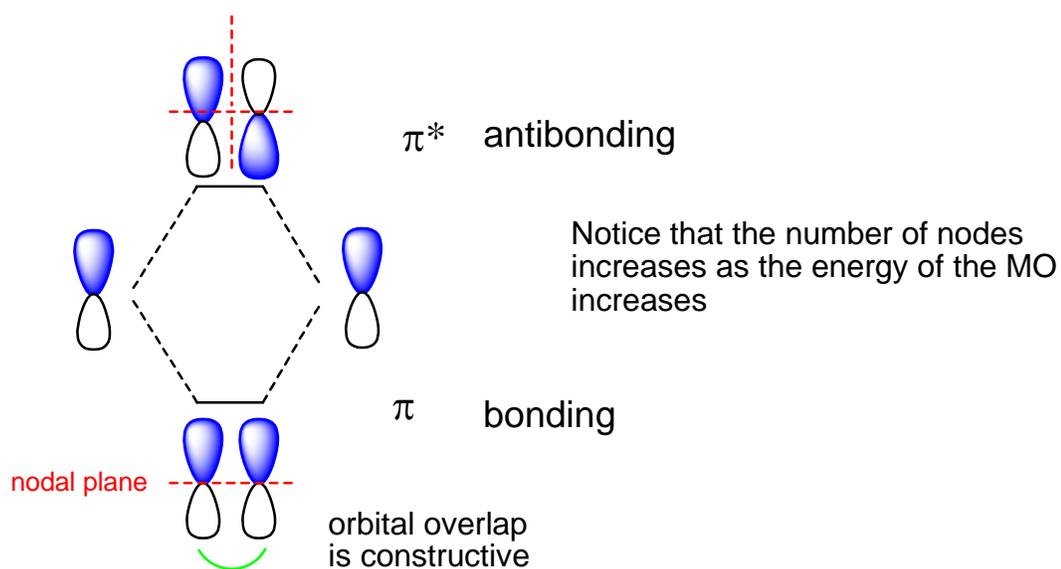As the energy of the MOs increase, the number of nodes increases

Orbital Interaction Diagram for the Hydrogen Molecule

A node is present in the antibonding MO

antibonding MO σ^* The antibonding orbital results from destructive interaction, i.e., overalp of orbitals that have opposite phase

E

1s orbitals (basis set)

The bonding orbital results from constructive interaction, i.e., overalp of orbitals that have the same phase

bonding MO σ

MO Diagram for Ethylene

The basis set is two unhybridized p-orbitals, one from each sp^2 carbon of the double bond

The asterisk is used to denote an antibonding MO

π^* antibonding

Notice that the number of nodes increases as the energy of the MO increases

π bonding

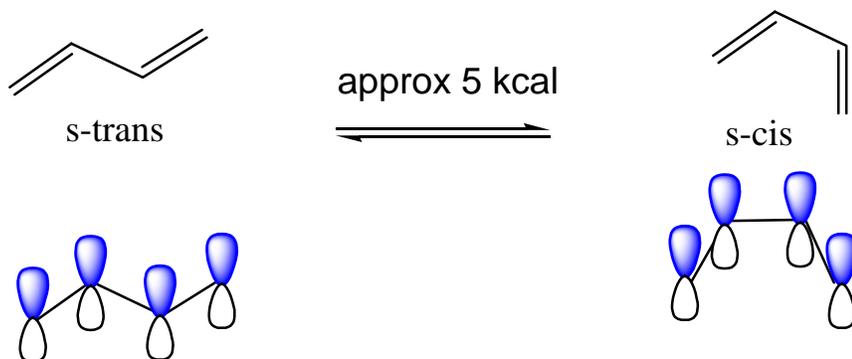nodal plane

orbital overlap is constructive

The little green arc is often used to indicate favorable overlap between lobes of various orbitals; notice this arc is absent in the antibonding orbital as expected since this is an unfavorable interaction (an interaction between p-orbitals of opposite phase)
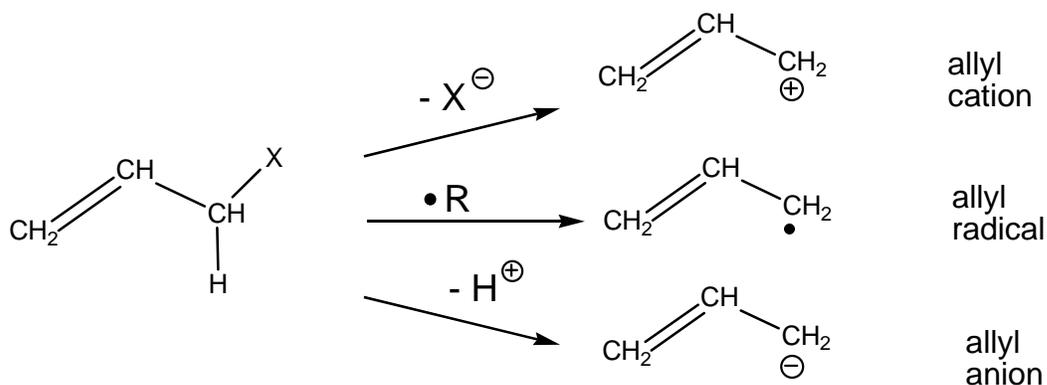
MO Diagram for 1,3-Butadiene

The basis set is 4 unhybridized p-orbitals or two "ethylene units"

π_4^* antibonding

π_3^* antibonding

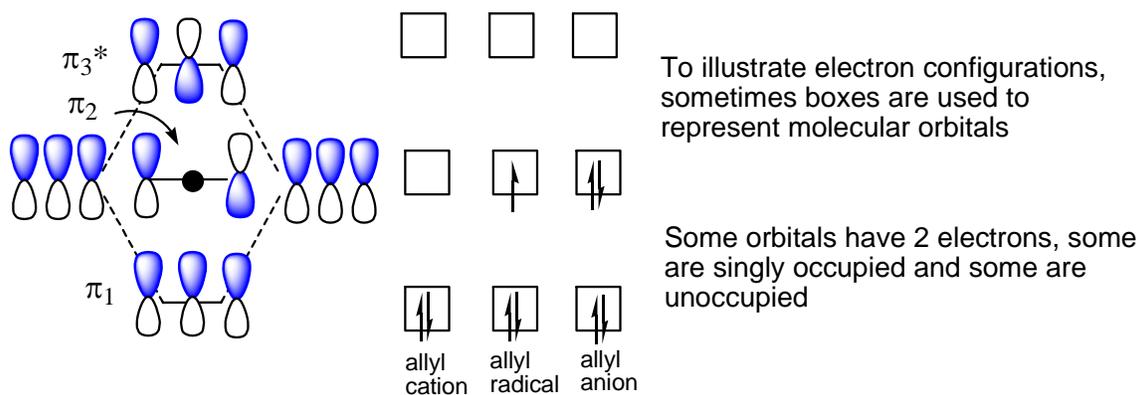The number of nodes increases
with increasing energy

π_2 bonding

π_1 bonding
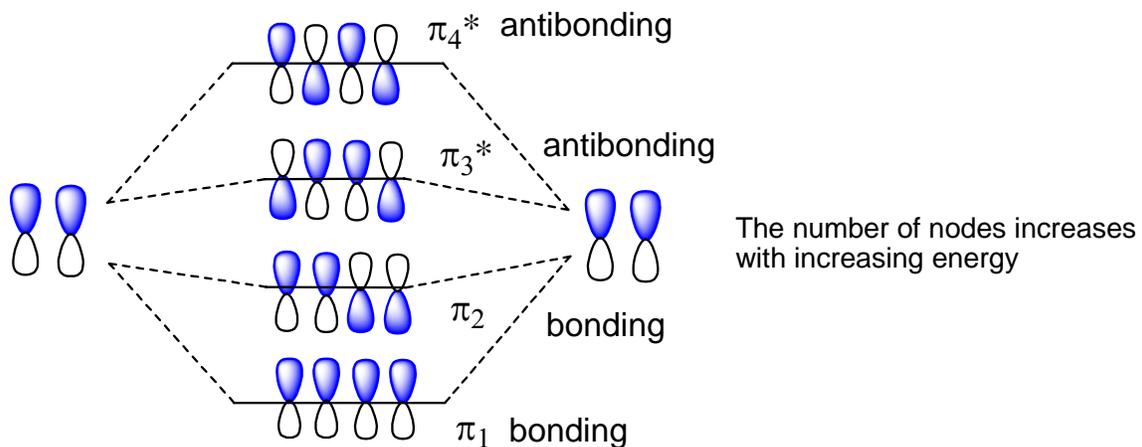
There are two conformations (single bond rotamers) that maintain the planar
topology of the butadiene system

s-trans

approx 5 kcal

s-cis

MO Diagram for the Allyl System

allyl
cation

allyl
radical

allyl
anion

The basis set is 3 p-orbitals, one from each carbon

π_3^*

π_2

π_1

allyl   allyl   allyl
cation radical anion

To illustrate electron configurations, sometimes boxes are used to represent molecular orbitals

Some orbitals have 2 electrons, some are singly occupied and some are unoccupied

Observe the symmetry of MO diagrams:

In butadiene and ethylene, an even number of p-orbitals produces the same number of π MO; 1/2 are bonding and 1/2 are antibonding

In the allyl system, an odd number of p-orbitals produces same the number of π MO; but the middle MO is nonbonding