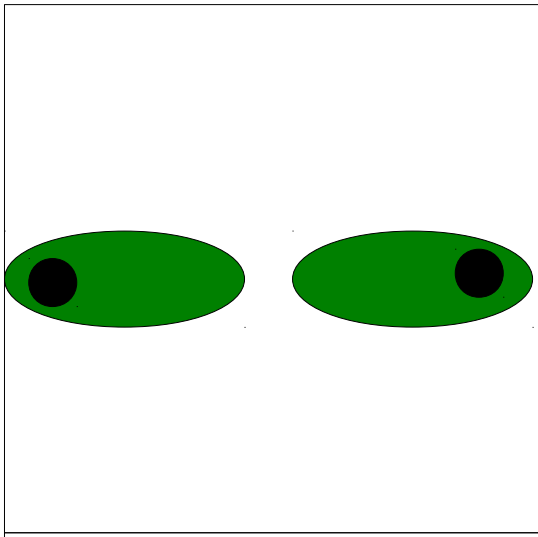
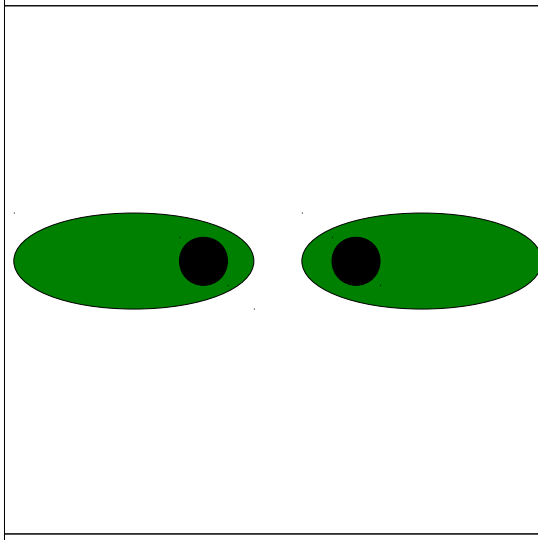
Definition of bonding characters of an MO

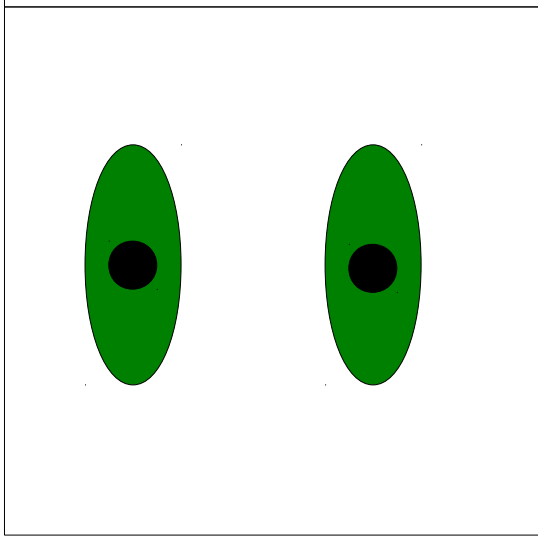
Nuclei repel each other, but are attracted to electrons.



bonding: **non-zero electronic density between the nuclei**. Each nucleus is attracted to the electrons, and so towards each other.



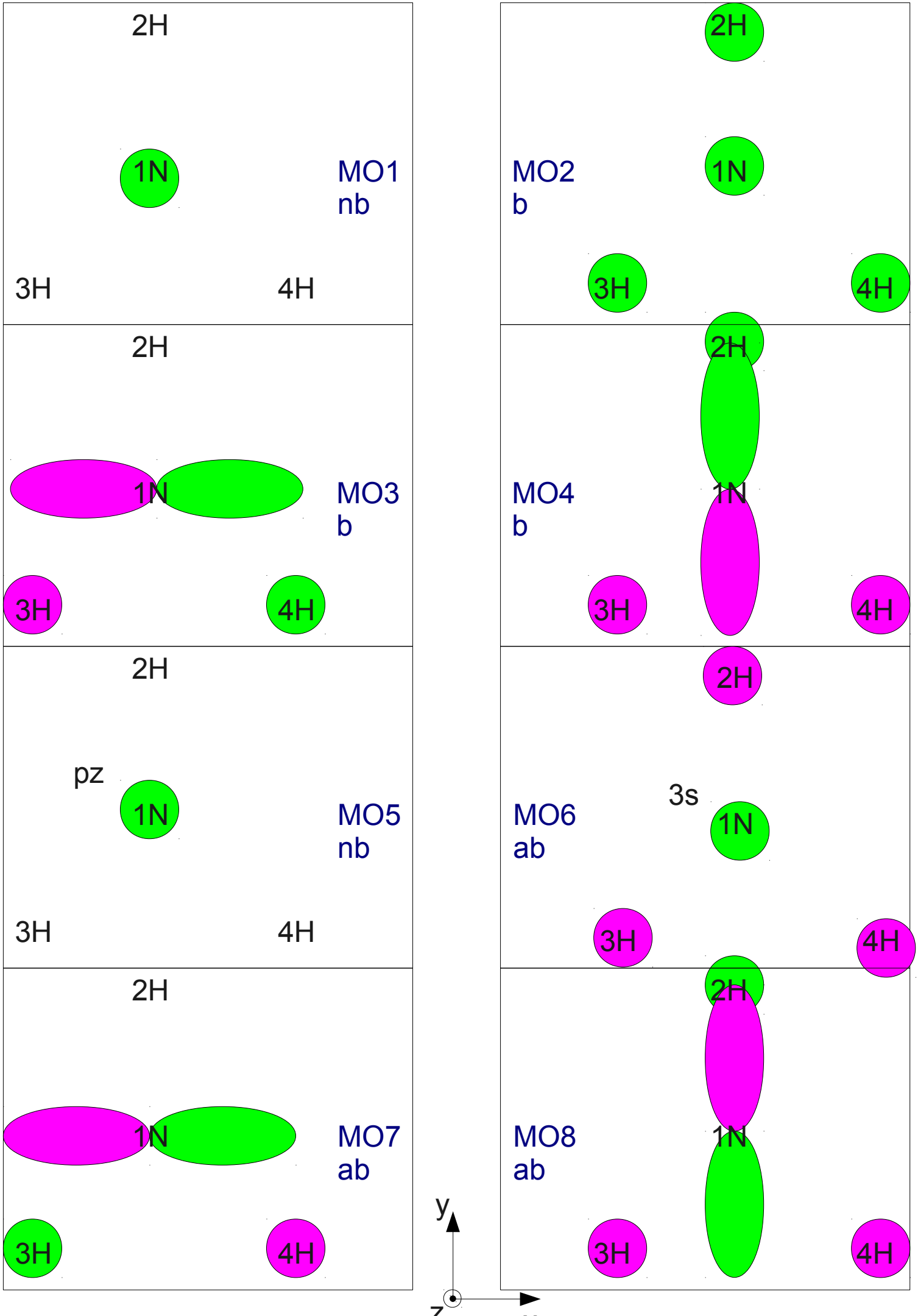
anti-bonding: **zero electronic density between the nuclei ("node"), and non-zero electronic density on either side of the nuclei**. Each nucleus is attracted most strongly to the electrons near it, and so away from each other.

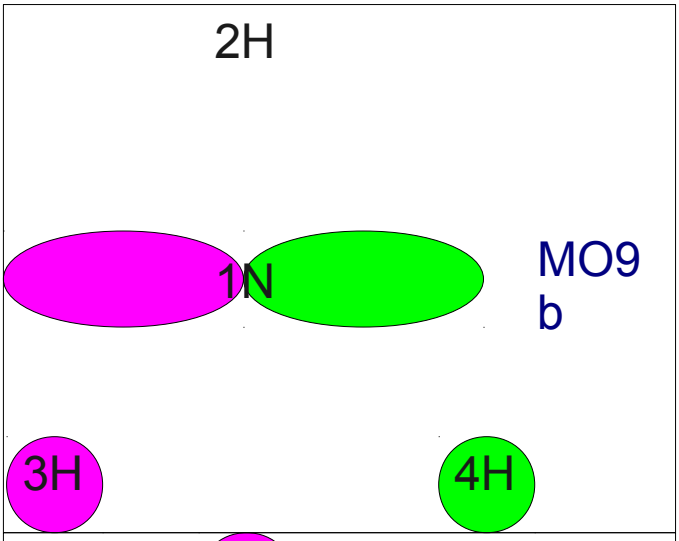


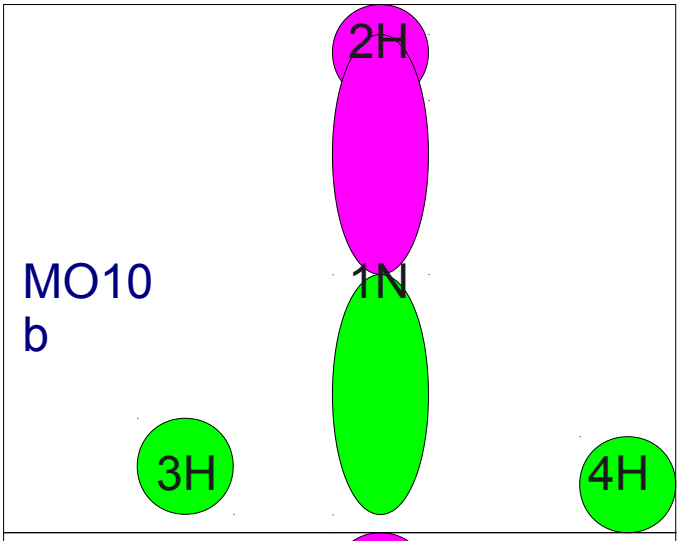
non-bonding: **zero electronic density between and on either side of the nuclei**. The electronic density associated with such an orbital neither causes the nuclei to attract or repel.

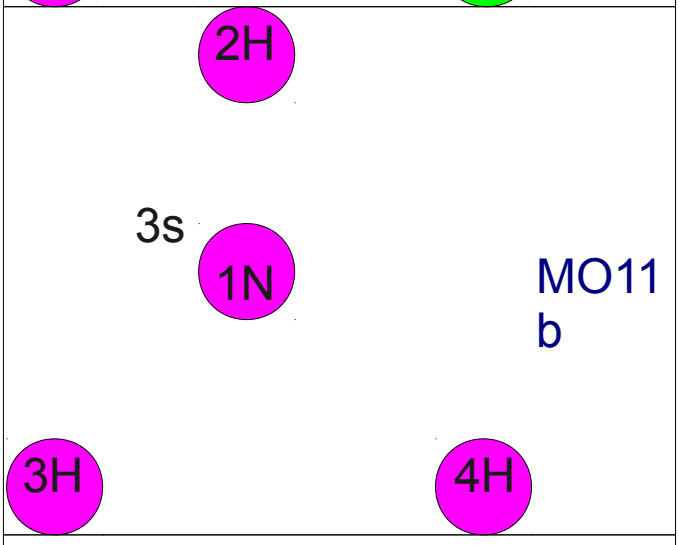
The bonding order (b.o.) is defined as the **difference between the number of occupied bonding MOs and occupied anti-bonding MOs**. For a closed shell system, this is equal to one-half of the difference between the number of bonding and anti-bonding electrons.(each occupied MO necessarily has occupation number 2).

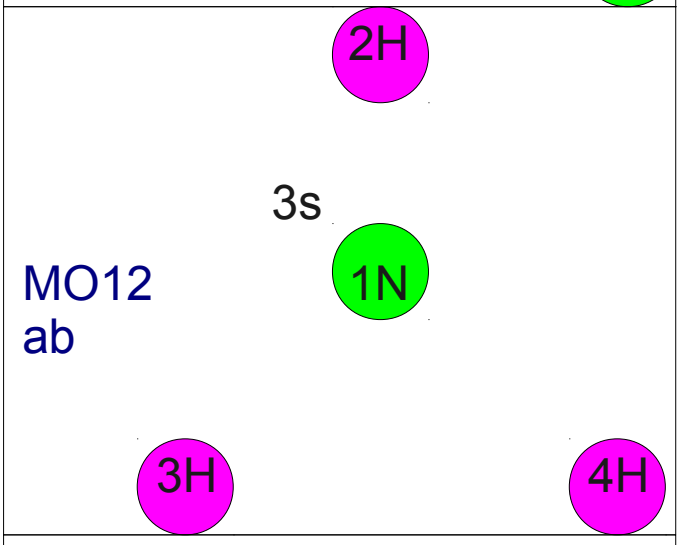
$$b.o. = \frac{n_b - n_{ab}}{2}$$

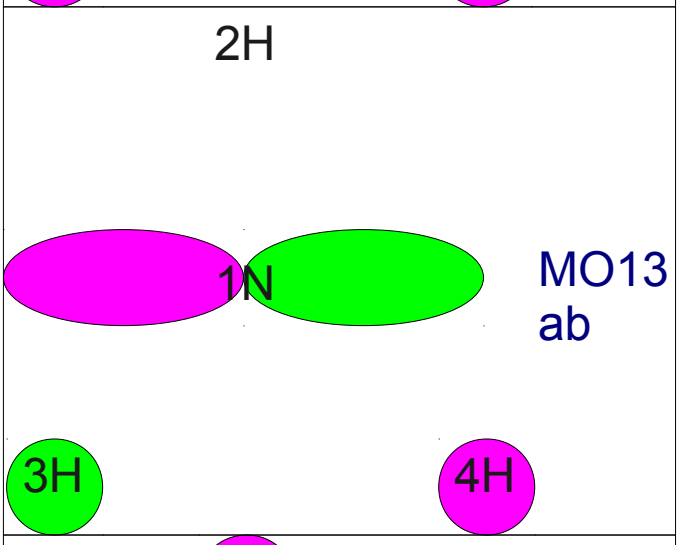

2H
1N
MO1
nb
3H
4H
2H
1N
MO2
b
3H
4H
2H
1N
MO3
b
3H
4H
2H
1N
MO4
b
3H
4H
2H
pz
1N
MO5
nb
3H
4H
2H
3s
1N
MO6
ab
3H
4H
2H
1N
MO7
ab
3H
4H
2H
1N
MO8
ab
3H
4H
y
z
x

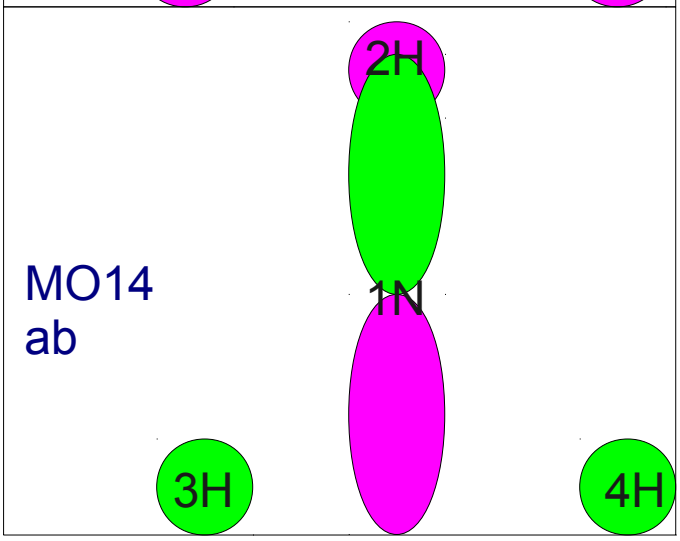


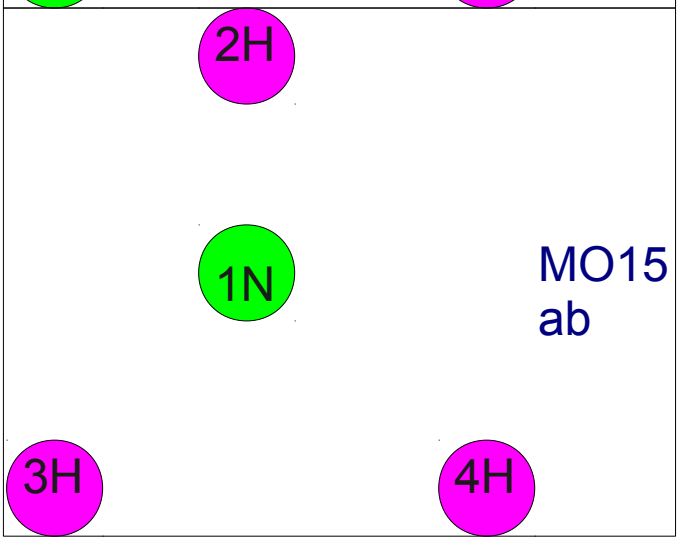












In MOs 5,6,8... sometimes we get such contributions as 1s(nH) – 2s(nH). Since 2s is more important for bonding, we disregard the contribution of the 1s.