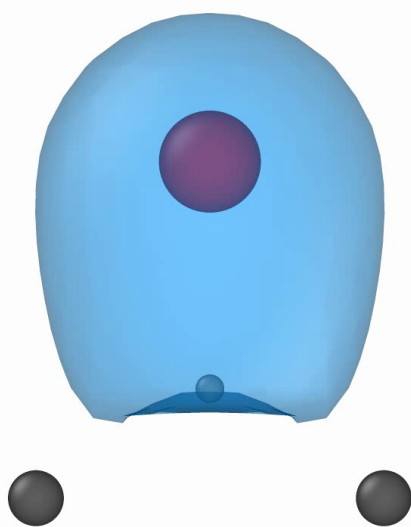


CPMD

SO STATE

CP2K

Orbital 0+1

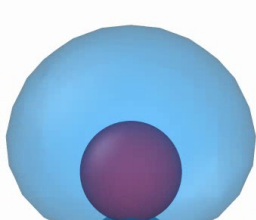


Orbital
1

Orbital 0+1

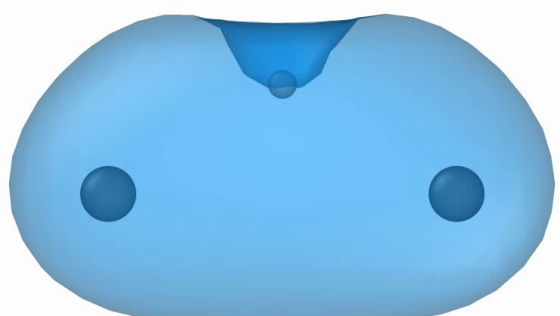
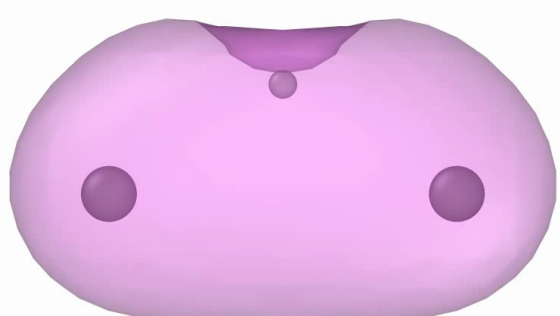
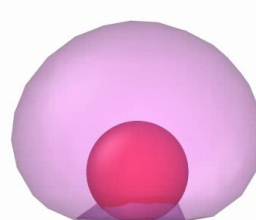


Orbital 1+1

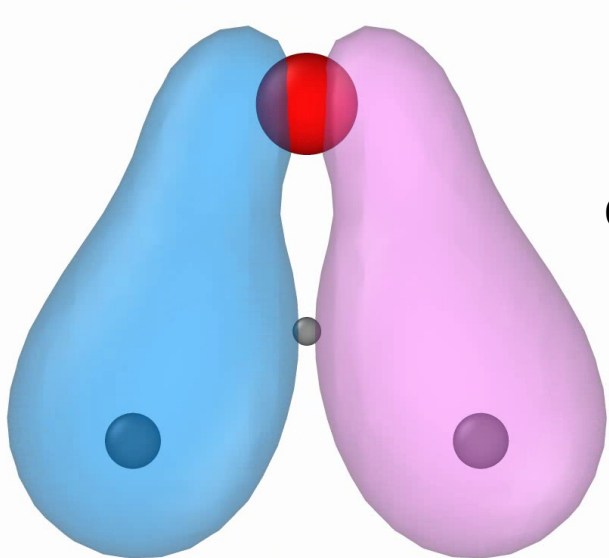


Orbital
2

Orbital 1+1

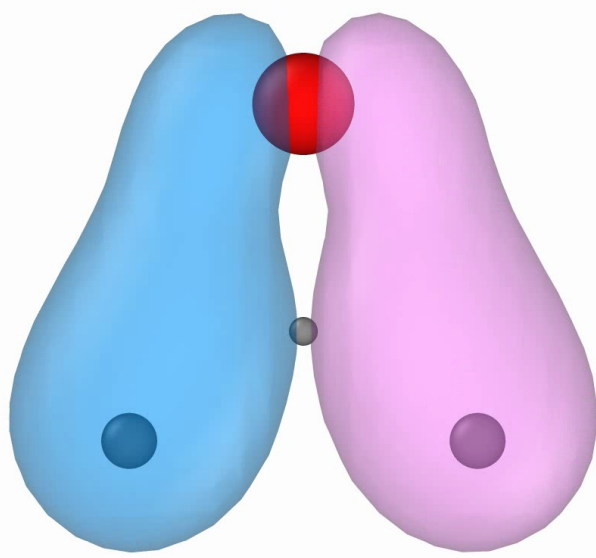


Orbital 2+1

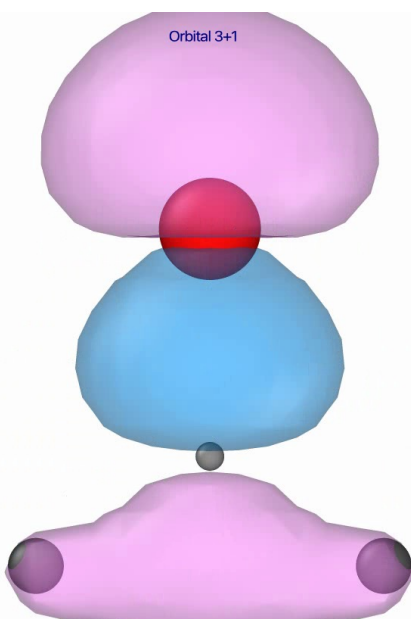


Orbital
3

Orbital 2+1

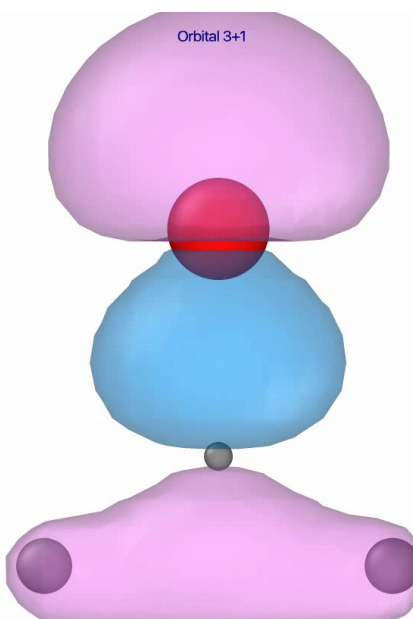


Orbital 3+1

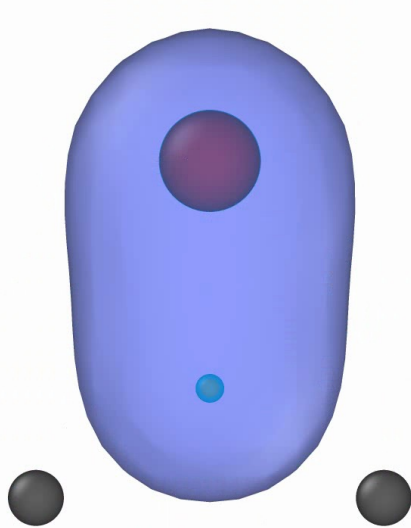


Orbital
4

Orbital 3+1

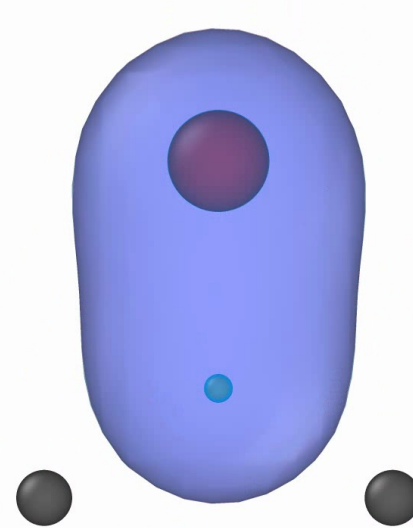


Orbital 4+1

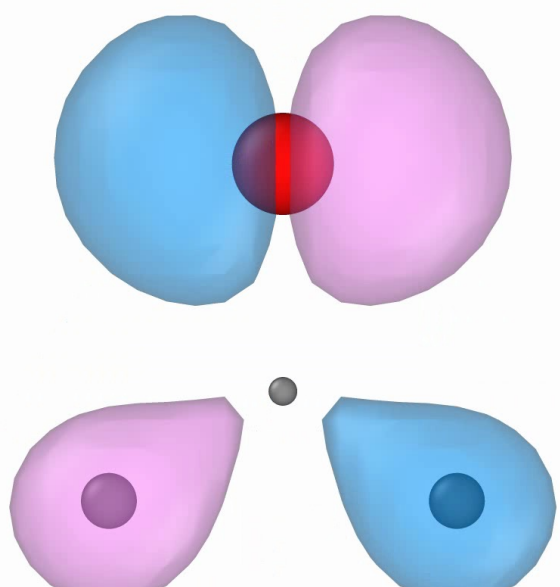


Orbital
5

Orbital 4+1

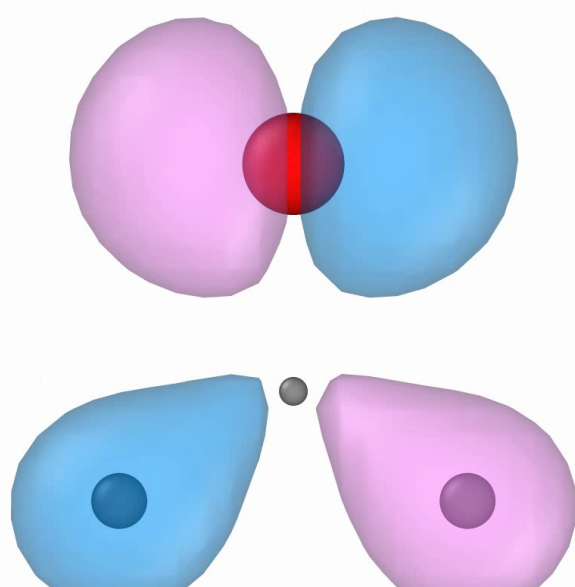


Orbital 5+1



Orbital
6
(HOMO)

Orbital 5+1

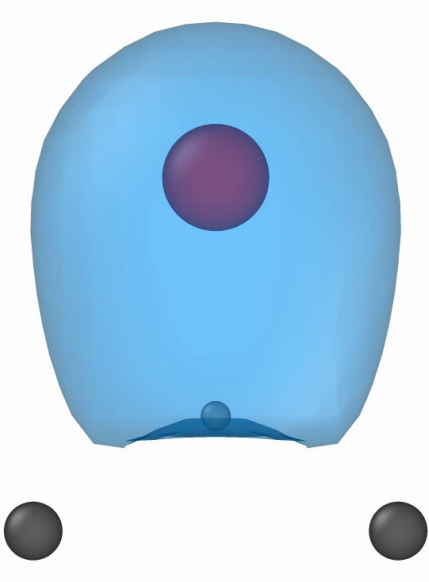


CPMD

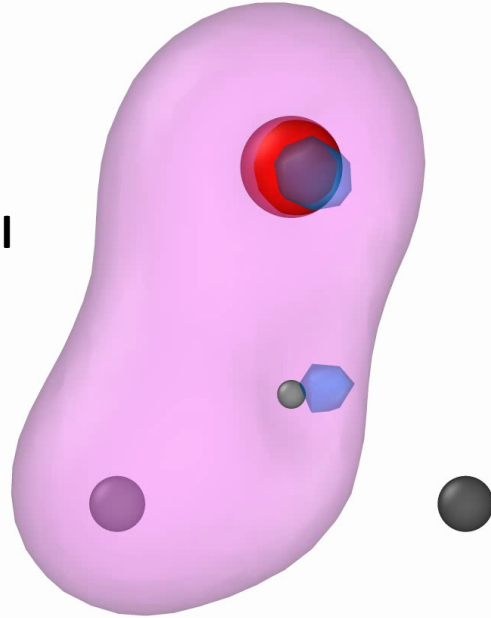
S1 STATE ROKS

CP2K

Orbital 0+1

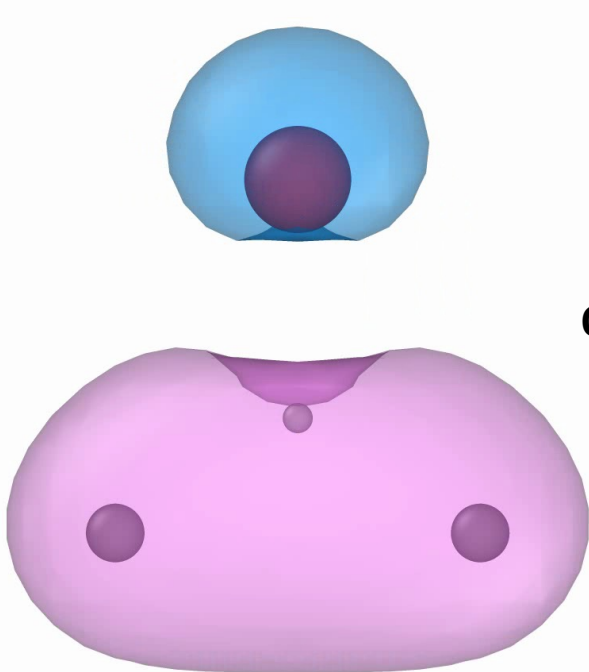


Orbital 0+1

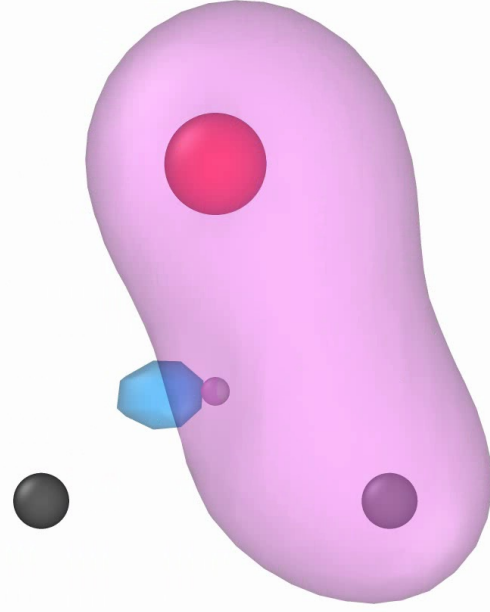


Orbital
1

Orbital 1+1

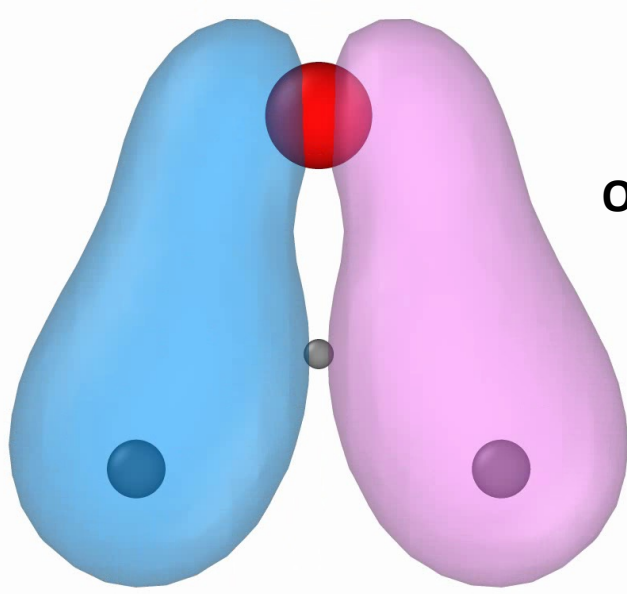


Orbital 1+1

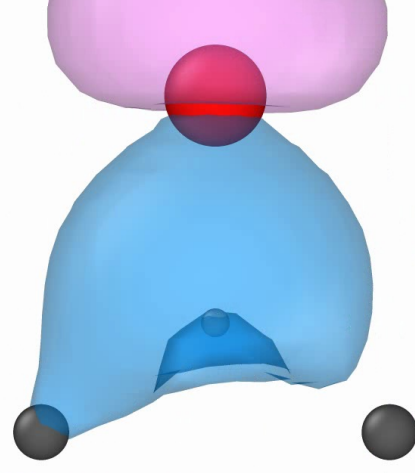


Orbital
2

Orbital 2+1

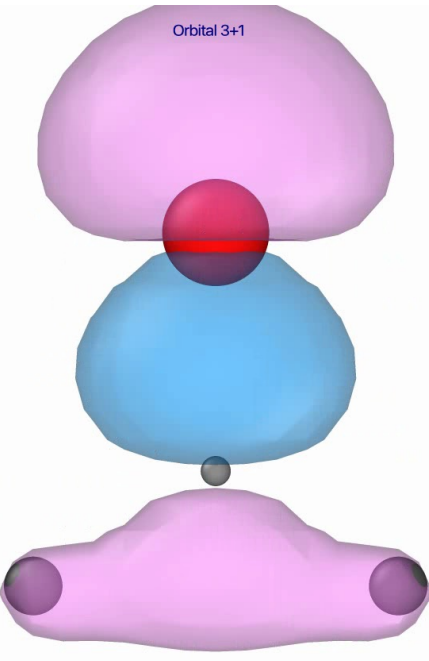


Orbital 2+1

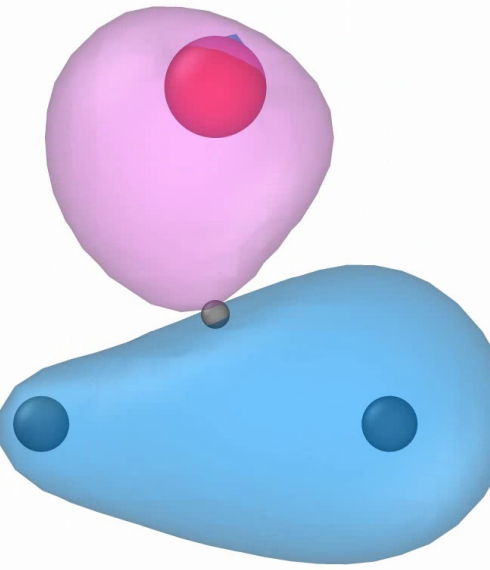


Orbital
3

Orbital 3+1

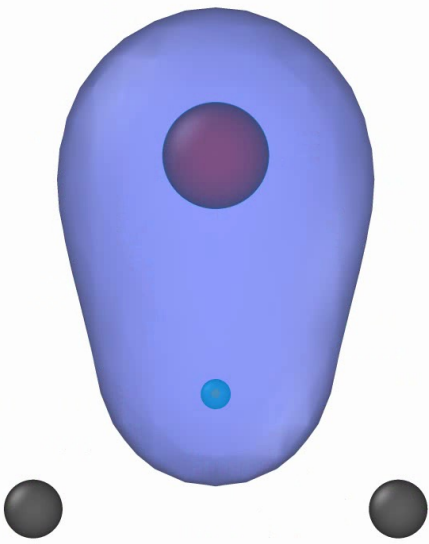


Orbital 3+1

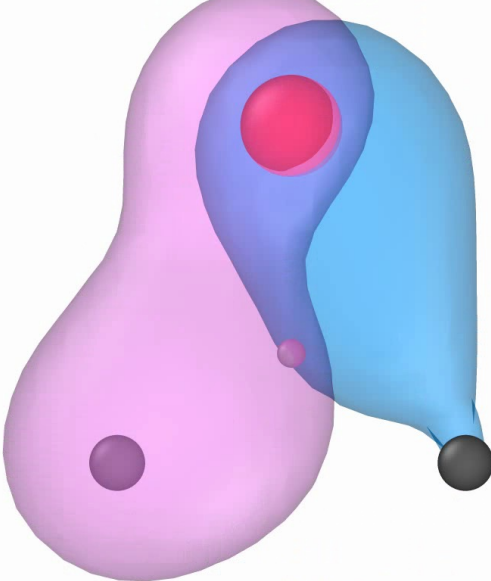


Orbital
4

Orbital 4+1

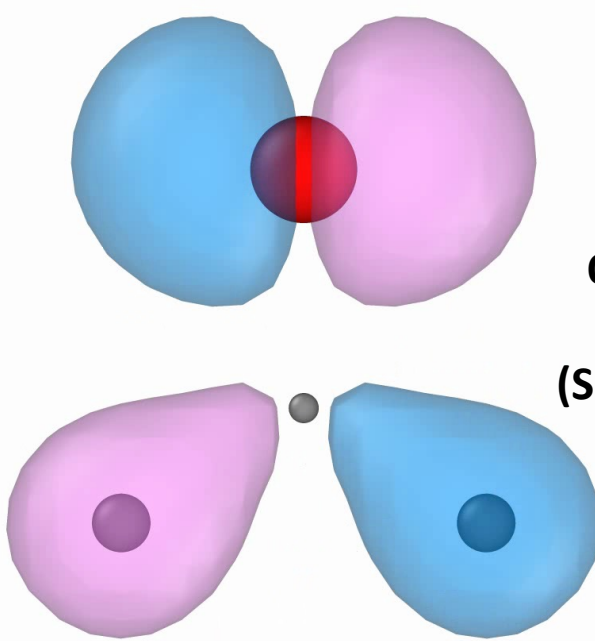


Orbital 4+1

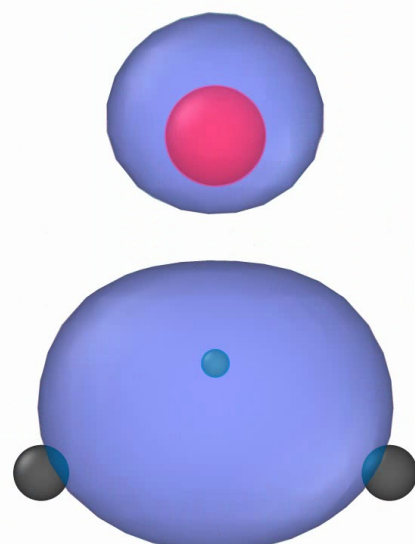


Orbital
5

Orbital 5+1

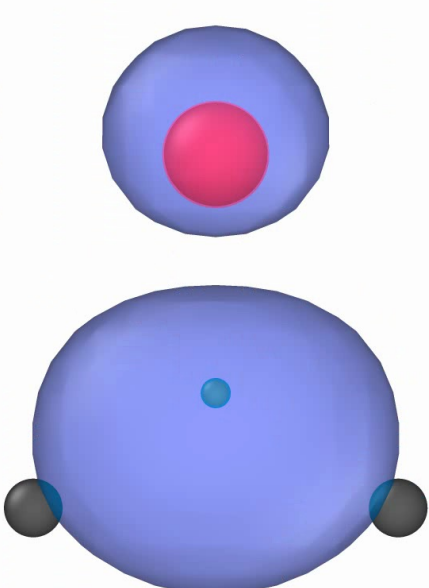


Orbital 5+1

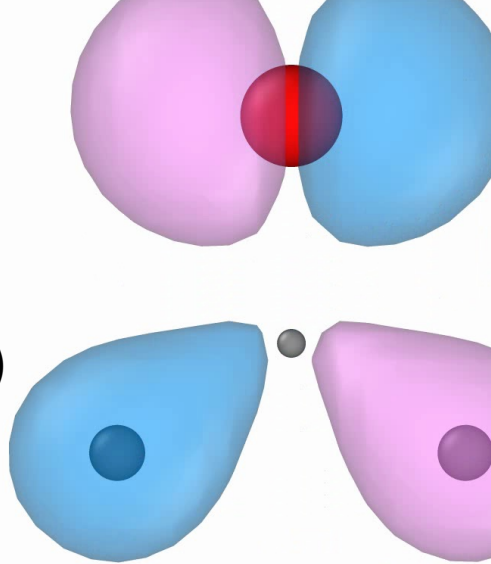


Orbital
6
(SOMO-1)

Orbital 6+1



Orbital 6+1



Orbital
7
(SOMO-2)