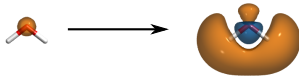


O 1s Excitation
in H₂O



Total Energy:

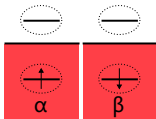
-76.3857 eh

-56.6582 eh

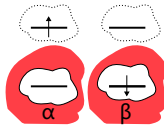
-56.4969 eh

-56.6583 eh

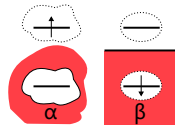
Level of
Relaxation
Included:



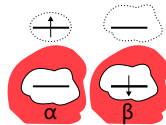
Ground State



Optimal h/p
+ full relaxation



Optimal h/p
+ α relaxation



Optimal h only
+ full relaxation