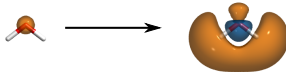


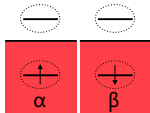
O 1s Excitation
in H₂O



Total Energy:

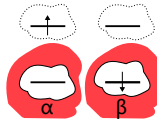
-76.3857 eh

Level of
Relaxation
Included:



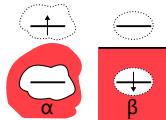
Ground State

-56.6582 eh



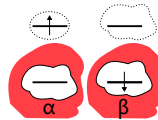
Optimal h/p
+ full relaxation

-56.4969 eh



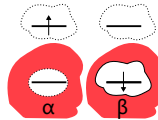
Optimal h/p
+ α relaxation

-56.6583 eh



Optimal h only
+ full relaxation

-76.1056 eh



Optimal p only
+ full relaxation