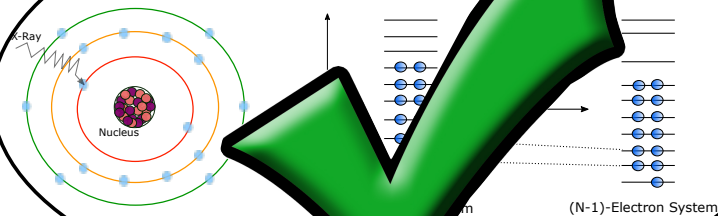
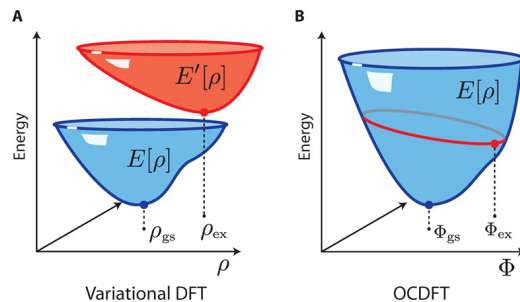
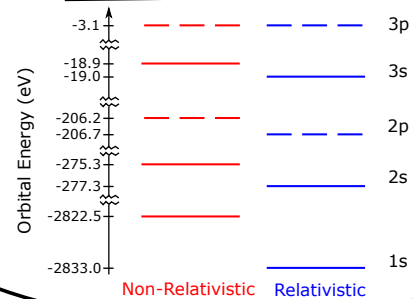


## Orbital Effects

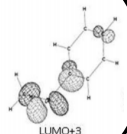
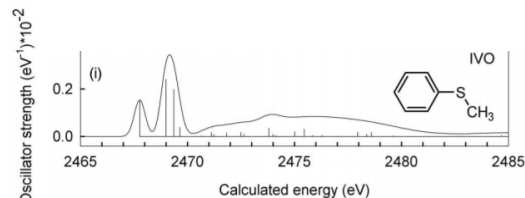


## Relativistic Effects



## Orthogonality Constrained Density Functional Theory

## Assigning Transitions



## Chemisorbed Complexes

