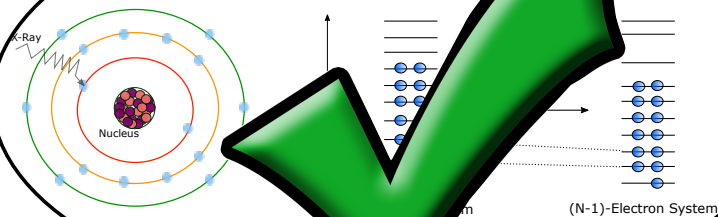
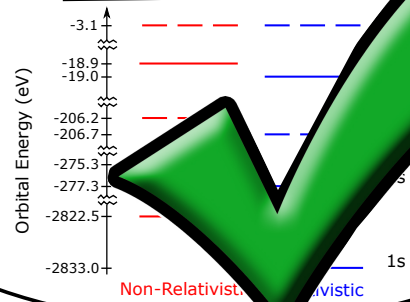


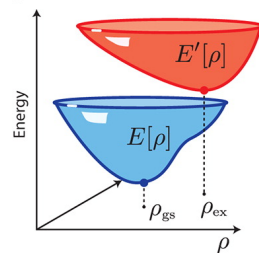
Orbital Effects



Relativistic Effects

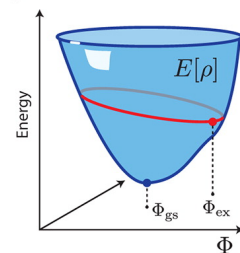


A



Variational DFT

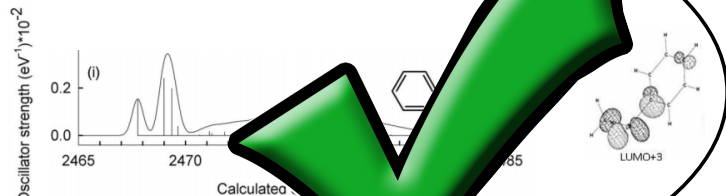
B



OCDFT

Orthogonality Constrained Density
Functional Theory

Assigning Transitions



Chemisorbed Complexes

