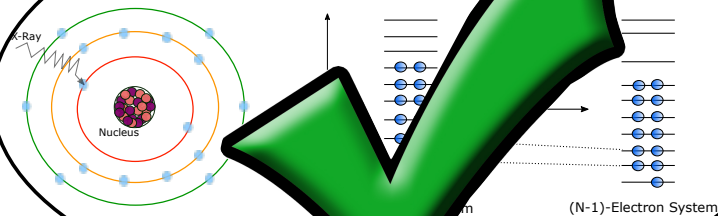
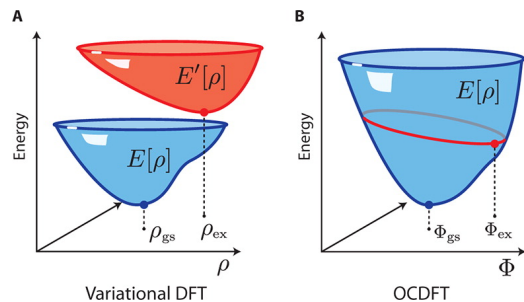
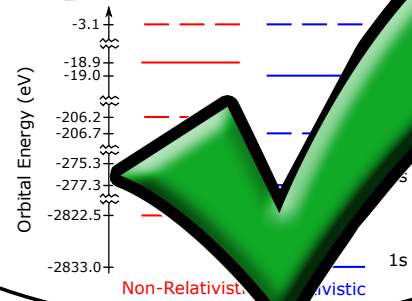


Orbital Effects

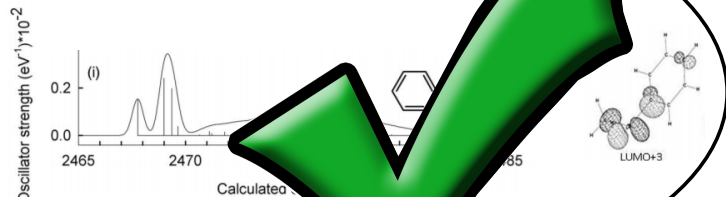


Relativistic Effects



Orthogonality Constrained Density Functional Theory

Assigning Transitions



Chemisorbed Complexes

