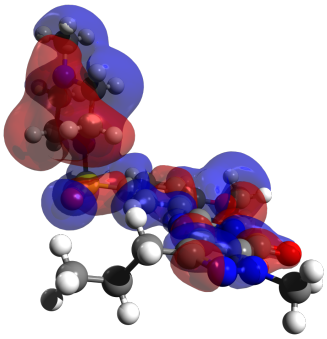
Density Functional Theory Calculations of Molecular Orbital Evolution During Chemical Reactions



Description: In this project we will focus on the calculation and visualization of the transformation of molecular orbitals following chemical reaction paths. A brief introduction will be given on background knowledge in chemistry, followed by hands-on tutorials on using the Atomic Simulation Environment (ASE) Python package to perform the calculations. Methods that use ensemble parallelization will then be explored to acceleration the turnaround time and throughput of the calculation.

Prerequisites: There are no formal prerequistes. Python proficiency is a plus but not required.