Chem279 Dr. Agrawal November 22, 2024

Chem 279 Assignment 5

In this assignment, we explored the analytical derivation of the CNDO/2 evaluation of energy for an H_2 molecule. My individual matrices are subpar but, for some reason, the final energy output vaguely matches the sample output?

Github: https://github.com/lkollmorgen/chem279_hw5