Hartree-Fock and MP2 Implementation Report

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Abstract

This report documents the implementation of the Hartree-Fock (HF) and Møller-Plesset perturbation theory (MP2) methods as developed in this repository. The focus is on the theoretical background, algorithmic details, and computational results obtained from the code.

1 Introduction

The Hartree-Fock method is a foundational approach in quantum chemistry for approximating the electronic structure of atoms and molecules. MP2 provides a post-Hartree-Fock correction to account for electron correlation effects. This report describes the implementation and results of these methods.

2 Theoretical Background

2.1 Hartree-Fock Method

Briefly describe the HF equations, self-consistent field (SCF) procedure, and the role of basis sets.

2.2 MP2 Correction

Summarize the MP2 energy correction and its significance in improving upon HF results.

3 Implementation Details

3.1 Code Structure

Outline the organization of the codebase and key modules.

3.2 Algorithms

Describe the main algorithms used for SCF convergence and MP2 energy calculation.

4 Results

Present sample results, such as total energies for test molecules, and compare HF and MP2 results.

5 Conclusion

Summarize findings and discuss possible improvements or future work.

References

List references to textbooks, articles, or documentation used.