SCFEnergyComputations

Welcome to the **SCFEnergyComputations** repository, where we delve into the fascinating world of quantum chemistry using the PySCF library. This repository hosts Jupyter notebooks that explore the computational aspects of the Self-Consistent Field (SCF) method, particularly focusing on energy calculations in molecular systems.

Overview

The content of this repository is centered around the implementation and analysis of SCF computations to determine molecular energies. We also explore Koopman's theorem to estimate ionization potentials and electron affinities from orbital energies obtained through SCF calculations.

Contents
- Step-by-step SCF energy calculations for a specified molecular system.
- Comparisons of computed SCF energies with experimental values.
- Applications of Koopman's theorem to estimate ionization potentials and electron affinities.
- Discussion on the impact of changing molecular geometries on system energies.

Getting Started

To get started with the notebooks in this repository, you will need to have Python installed along with the PySCF library and other scientific computing tools such as NumPy and Matplotlib. Follow these steps to set up your environment:

1. **Install Python**: Ensure that Python 3.x is installed on your system. You can download it from [python.org](https://www.python.org/downloads/).

2. **Set up a virtual environment** (optional but recommended):
   ```bash
   python -m venv venv
   source venv/bin/activate  # On Windows use `venv\Scripts\activate`
   ```

3. **Install required packages**:
   ```bash
   pip install numpy matplotlib pyscf
   ```

4. **Clone this repository**:
   ```bash
   git clone https://github.com/yourusername/SCFEnergyComputations.git
   cd SCFEnergyComputations
   ```

5. **Launch Jupyter Notebook**:
   ```bash
   jupyter notebook
   ```

Navigate to the notebook `UE06.ipynb` to start exploring.