Computational Chemistry Input Builder

The Computational Chemistry Input Builder is a user-friendly graphical user interface (GUI) application developed using Python's Tkinter library. The primary objective of this project is to streamline the creation of input files for computational chemistry software, thereby making the process more accessible and efficient for users with varying levels of expertise. Traditionally, creating these input files involves manually editing text files, which can be both time-consuming and prone to errors. This project addresses these challenges by providing an intuitive interface that allows users to configure various parameters dynamically and generate the necessary input files with ease.

The current methods for generating input files for computational chemistry software often require a deep understanding of the specific syntax and parameters involved, which can be a barrier for many users. Existing tools may not offer the flexibility and user-friendly interface needed to reduce the complexity of this task. The Computational Chemistry Input Builder, however, offers a solution by allowing users to select and configure parameters such as SCFMETH, LVL, CHARGE, SPIN, MEMORY, MEMDDI, and BASIS through a series of drop-down menus. This approach minimizes the risk of errors and significantly enhances the user experience.

The design and development of the application involved several key components. Using Tkinter, the project includes dynamically created option menus for parameter selection, ensuring that users can easily choose from predefined lists. Additionally, the application features buttons for importing geometry files, generating and displaying the input file content, saving the generated files, and submitting the input. The ability to import geometry files is particularly useful, as it allows users to integrate their existing data seamlessly. The generated content is displayed in a text area within the application, providing users with an immediate preview of the input file.

Technically, the application manages parameter values through a dictionary, which is updated based on user selections. This ensures that the input file content accurately reflects the chosen parameters. The file handling capabilities, including importing geometry files and saving the generated input files, add to the application's functionality and user-friendliness. The content generation process combines the parameter values and geometry content into a formatted input file template, which is then displayed for review and can be saved for future use.

The outcome of this project is a tool that significantly simplifies the process of creating input files for computational chemistry software. By offering a user-centric design, the Computational Chemistry Input Builder reduces the likelihood of errors and improves the overall efficiency of the input file generation process. This tool is particularly beneficial for users who are not familiar with the detailed syntax required for these files, making computational chemistry more accessible to a broader audience.

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