Project Report: Molecule Analysis Tool Using Python

Project Title

Molecule Analysis Tool Using Tkinter and Matplotlib

Objective

To develop a graphical user interface (GUI) application that analyzes molecular structure data, calculates bond potentials, and visualizes molecular properties using Python.

Technologies Used

- Python 3
- NumPy for numerical computations
- Matplotlib for plotting
- Tkinter for GUI interface
- math module for distance calculations

Functionalities

- Load molecule structure from XYZ file
- Calculate bond distances between atom pairs
- Compute bond potential using harmonic approximation
- Plot bond potential vs. equilibrium bond length
- Display molecular geometry in text format
- User-friendly help section and exit controls

Code Description

The application loads molecular coordinates from an .xyz file and allows the user to interact via buttons. Users can select atom pairs to calculate distances and bond potentials. A bond potential graph can be plotted

using default parameters. The GUI is styled using basic Tkinter customization.

Graphical Elements

The program includes labeled buttons, message boxes for displaying values, and styled GUI using custom colors and fonts for better UX.

Applications

- Educational tool for computational chemistry
- Visualizing molecular bond behavior
- Quick bond potential calculations for small molecules

Conclusion

This project demonstrates a well-rounded integration of data analysis, visualization, and GUI interaction. It serves as a simple yet powerful tool for students and researchers in computational chemistry, providing insight into molecular bonds and behavior in an interactive way.