InteractiveMDTools

Welcome to **InteractiveMDTools**, a repository designed for researchers, educators, and students interested in exploring the dynamics of molecules through interactive simulations. This repository provides a suite of tools to visualize and understand Morse potentials and harmonic bond potentials using Python-based simulations.

Features

- **Morse Potential Visualization**: Interactive widgets to adjust parameters like depth \(D\), equilibrium bond length \(r_0\), and stiffness \(alpha\) to see their effects on the potential curve.

- **Harmonic Bond Potential**: Tools to visualize and tweak the spring constant \(k\) and equilibrium position \(r_0\) for harmonic oscillators, representing bonded interactions.

- **Molecular Dynamics Simulations**: Basic setup for running molecular dynamics simulations with the ASE library to observe molecular behavior over time.

- **Energy Visualization**: Plotting tools to track potential, kinetic, and total energy of a system during simulations.

Installation

To get started with **InteractiveMDTools**, you will need to install several Python libraries. You can install these libraries using `pip`:

```bash
pip install numpy matplotlib ase ipywidgets
```

Ensure you have Python installed on your system (Python 3.7 and above is recommended). You can verify your Python version by running:

```bash
python --version
```

Usage

To use the tools provided in this repository, simply clone the repo and launch the Jupyter notebooks:

```bash
git clone https://github.com/your-username/InteractiveMDTools.git
cd InteractiveMDTools
```

jupyter notebook
```

Navigate to the desired notebook and follow the interactive prompts to adjust simulation parameters.
```