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Project Structure:

molecular_simulation_code/

optimizer.py # Core optimization logic (LJ potential + basin-hopping)

visualization.py # Cluster plotting, energy evolution, animation

io_utils.py # XYZ saving, trajectory output

main.py # Run script to launch optimization and generate results

outputs/ # Saved figures, XYZ files, GIF animations

Python package dependencies:

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numpy

scipy

matplotlib
```

How to Run the Code:

1. Install Dependencies:

Make sure Python 3.8+ is installed. Then run:

pip install -r requirements.txt

2. Run the Optimization:

python main.py

This will:

- Optimize the LJ cluster (default: LJ38)

- Save final XYZ structure

3. Output Files (saved in outputs/):

- LJ38_best_energy.png Energy vs. Step plot
- LJ38_final.xyz Final optimized coordinates
- LJ38_trajectory.xyz Trajectory of accepted steps
- LJ38_animation.gif Structure evolution animation

Configuration:

You can modify main.py to:

- Change number of atoms (e.g., N = 38)
- Adjust number of optimization steps
- Enable or disable visualization

Contact:

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