MINI_potential

September 26, 2024
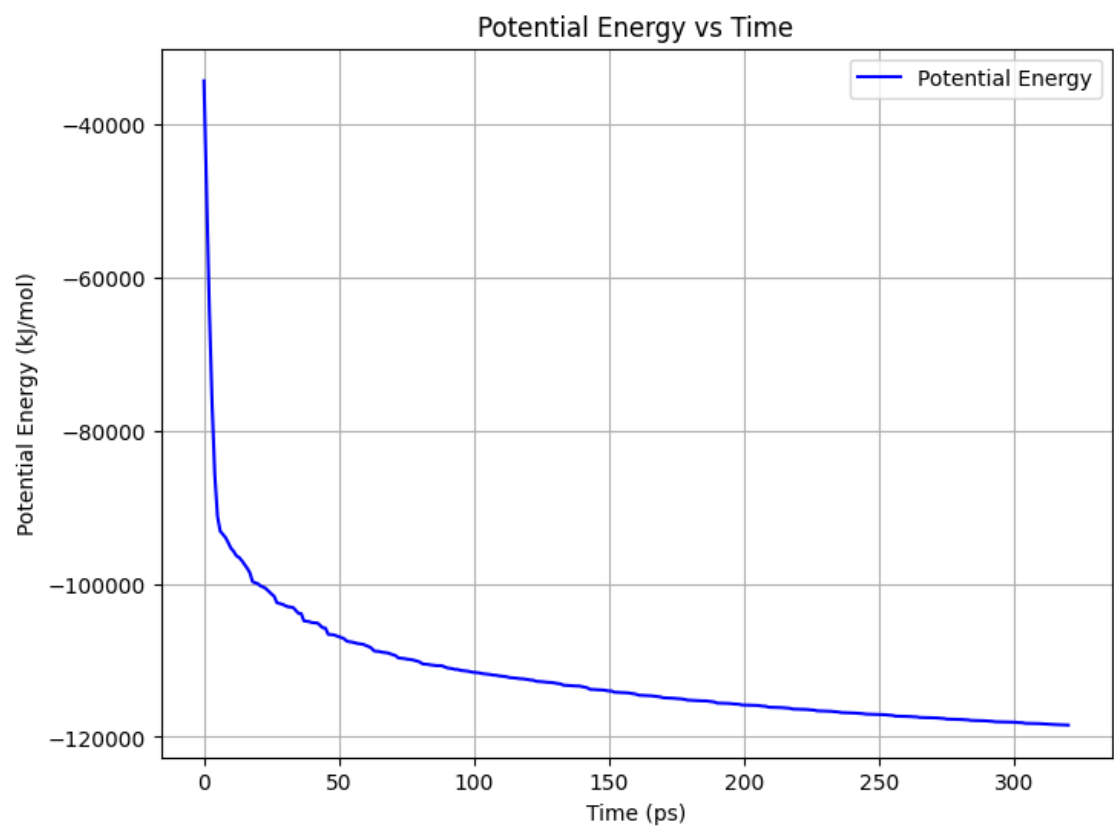
```python
[4]: import numpy as np
     import matplotlib.pyplot as plt

     #    .xvg       #   @
     def read_xvg(filename):
         data = []
         with open(filename, 'r') as file:
             for line in file:
                 if not line.startswith(('#', '@')):
                     data.append([float(x) for x in line.split()])
         return np.array(data)

     #      WSL
     data = read_xvg('./potential.xvg')

     #
     time = data[:, 0]
     potential_energy = data[:, 1]

     #   Potential Energy vs Time
     plt.figure(figsize=(8, 6))
     plt.plot(time, potential_energy, label='Potential Energy', color='b')
     plt.xlabel('Time (ps)')
     plt.ylabel('Potential Energy (kJ/mol)')
     plt.title('Potential Energy vs Time')
     plt.grid(True)
     plt.legend()
     plt.show()
```

Potential Energy vs Time

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