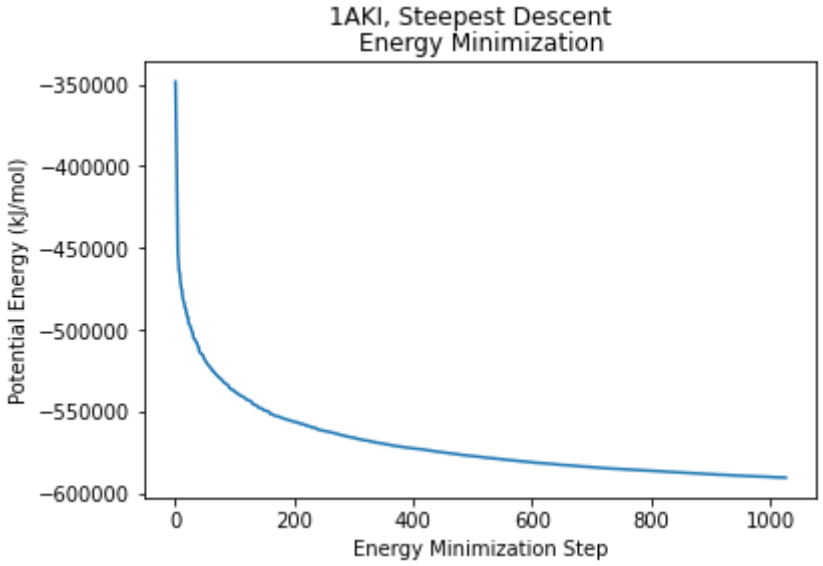
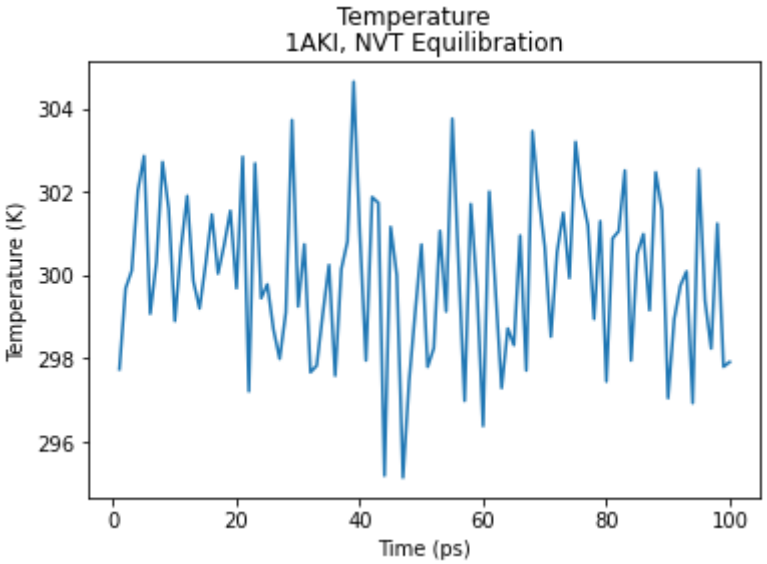
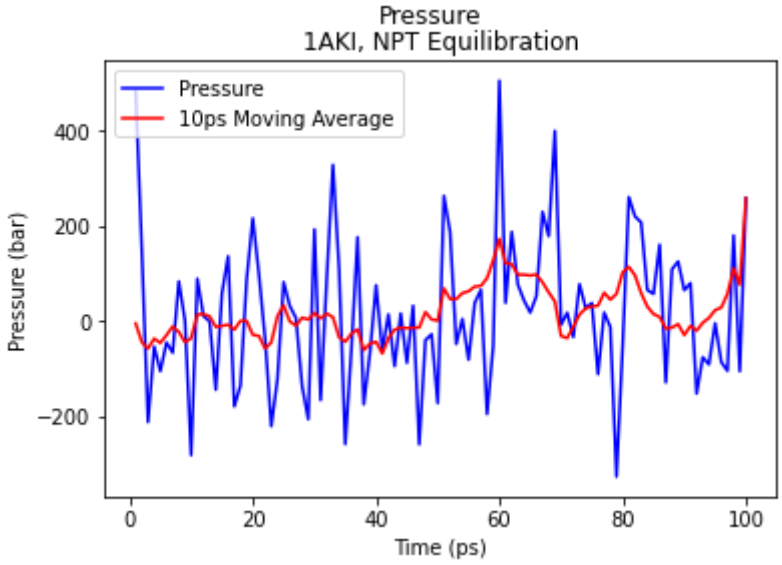
In [2]:
```
import matplotlib.pyplot as plt
import numpy as np

# open potential.xvg file and read from line 25
with open('potential.xvg', 'r') as f:
    lines = f.readlines()[25:]
    lines = [line.split() for line in lines]
    lines = [[float(i) for i in line] for line in lines]

# plot potential energy (kJ/mol) vs energy minimization step  graph
plt.plot([line[0] for line in lines], [line[1] for line in lines])
plt.xlabel('Energy Minimization Step')
plt.ylabel('Potential Energy (kJ/mol)')
plt.title('Energy Minimization')
plt.suptitle('1AKI, Steepest Descent')
plt.show()
```



In [3]:
```
# open temperature.xvg file and read from line 25
with open('temperature.xvg', 'r') as f:
    lines = f.readlines()[25:]
    lines = [line.split() for line in lines]
    lines = [[float(i) for i in line] for line in lines]

# plot temperature (K) vs time (ps) graph
plt.plot([line[0] for line in lines], [line[1] for line in lines])
plt.xlabel('Time (ps)')
plt.ylabel('Temperature (K)')
plt.title('1AKI, NVT Equilibration')
plt.suptitle('Temperature')
plt.show()
```



In [6]:
```
# open pressure.xvg file and read from line 25
with open('pressure.xvg', 'r') as f:
    lines = f.readlines()[25:]
    lines = [line.split() for line in lines]
    lines = [[float(i) for i in line] for line in lines]

# plot pressure (bar) vs time (ps) graph and 10ps moving average
# add legend
plt.plot([line[0] for line in lines], [line[1] for line in lines], color='b
plt.plot([line[0] for line in lines], [np.mean([line[1] for line in lines[i
plt.xlabel('Time (ps)')
plt.ylabel('Pressure (bar)')
plt.title('1AKI, NPT Equilibration')
plt.suptitle('Pressure')
plt.legend()
plt.show()
```



In [7]:
```
# open density.xvg file and read from line 25
with open('density.xvg', 'r') as f:
    lines = f.readlines()[25:]
    lines = [line.split() for line in lines]
    lines = [[float(i) for i in line] for line in lines]

# plot density (kg/m^3) vs time (ps) graph and 10ps moving average
# add legend
plt.plot([line[0] for line in lines], [line[1] for line in lines], color='b
plt.plot([line[0] for line in lines], [np.mean([line[1] for line in lines[i
plt.xlabel('Time (ps)')
plt.ylabel('Density (kg/m^3)')
plt.title('1AKI, NPT Equilibration')
plt.suptitle('Density')
plt.legend()
plt.show()
```