

## Molecular Dynamics Simulation Report

Optimized Lattice Parameter:  $5.2809 \times 10^{-10}$  m

Melting Point: 190 K

Boiling Point: 195 K

Total Runtime: 50.40 seconds

Best Verlet Algorithm: Velocity-Verlet (Adaptive)

Best Time Step:  $1.00 \times 10^{-14}$  s

Reason: Lowest average potential energy ( $-1.31 \times 10^{-20}$  J) and minimal energy drift ( $1.46 \times 10^{-25}$  J) during preliminary simulation.

