

# Molecular Dynamics Simulation Report

Optimized Lattice Parameter:  $5.2823 \times 10^{-10}$  m

Melting Point: 85 K

Boiling Point: 160 K

Total Runtime: 5702.03 seconds

Best Verlet Algorithm: Leapfrog Verlet (Adaptive)

Best Time Step:  $1.00 \times 10^{-16}$  s

Reason: Lowest average potential energy ( $-1.29 \times 10^{-20}$  J) and minimal energy drift ( $2.86 \times 10^{-24}$  J) during preliminary simulation.

