

# Molecular Dynamics Simulation Report

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

Melting Point: 95 K

Boiling Point: 105 K

Total Runtime: 756.01 seconds

Best Verlet Algorithm: Velocity-Verlet (Adaptive)

Best Time Step:  $1.00 \times 10^{-15}$  s

Reason: Lowest average potential energy ( $-1.29 \times 10^{-20}$  J) and minimal energy drift ( $8.13 \times 10^{-23}$  J) during preliminary simulation.

