

# Molecular Dynamics Simulation Report

Optimized Lattice Parameter:  $5.2756 \times 10^{-10}$  m

Melting Point: 190 K

Boiling Point: 195 K

Total Runtime: 650.04 seconds

Best Verlet Algorithm: Standard Verlet (Adaptive)

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

Reason: Lowest average potential energy ( $-1.21 \times 10^{-20}$  J) and minimal energy drift ( $4.35 \times 10^{-22}$  J) during preliminary simulation.

