

## Molecular Dynamics Simulation Report

Optimized Lattice Parameter:  $5.2727 \times 10^{-10}$  m

Melting Point: 155 K

Boiling Point: 160 K

Total Runtime: 906.88 seconds

Best Verlet Algorithm: Standard Verlet (Adaptive)

Best Time Step:  $1.00 \times 10^{-17}$  s

Reason: Lowest average potential energy ( $-1.41 \times 10^{-18}$  J) and minimal energy drift ( $2.17 \times 10^{-22}$  J) during preliminary simulation.

