

Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2742×10^{-10} m

Melting Point: 90 K

Boiling Point: 165 K

Total Runtime: 3768.88 seconds

Best Verlet Algorithm: Velocity-Verlet (Adaptive)

Best Time Step: 5.00×10^{-15} s

Reason: Lowest average potential energy (-1.41×10^{-18} J) and minimal energy drift (2.20×10^{-23} J) during preliminary simulation.

