

Molecular Dynamics Simulation Report

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

Melting Point: 150 K

Boiling Point: 155 K

Total Runtime: 4605.25 seconds

Best Verlet Algorithm: Velocity-Verlet (Adaptive)

Best Time Step: 1.00×10^{-16} s

Reason: Lowest average potential energy (-1.41×10^{-18} J) and minimal energy drift (8.22×10^{-24} J) during preliminary simulation.

