

Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2823×10^{-10} m

Melting Point: 95 K

Boiling Point: 175 K

Total Runtime: 2106.50 seconds

Best Verlet Algorithm: Leapfrog Verlet (Adaptive)

Best Time Step: 1.00×10^{-15} s

Reason: Lowest average potential energy (-1.29×10^{-20} J) and minimal energy drift (1.75×10^{-23} J) during preliminary simulation.

