

Molecular Dynamics Simulation Report

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

Melting Point: 90 K

Boiling Point: 110 K

Total Runtime: 1977.45 seconds

Best Verlet Algorithm: Velocity-Verlet (Adaptive)

Best Time Step: 1.00×10^{-15} s

Reason: Lowest average potential energy (-1.22×10^{-20} J) and minimal energy drift (4.50×10^{-23} J) during preliminary simulation.

