

Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2809×10^{-10} m

Melting Point: 140 K

Boiling Point: 170 K

Total Runtime: 262.13 seconds

Best Verlet Algorithm: Velocity-Verlet (Adaptive)

Best Time Step: 1.00×10^{-15} s

Reason: Lowest average potential energy (-1.41×10^{-18} J) and minimal energy drift (6.66×10^{-24} J) during preliminary simulation.

