

Molecular Dynamics Simulation Report

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

Melting Point: 195 K

Boiling Point: 200 K

Total Runtime: 222.52 seconds

Best Verlet Algorithm: Velocity-Verlet (Adaptive)

Best Time Step: 1.00×10^{-14} s

Reason: Lowest average potential energy (-1.22×10^{-20} J) and minimal energy drift (2.21×10^{-25} J) during preliminary simulation.

