

Molecular Dynamics Simulation Report

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

Melting Point: 75 K

Boiling Point: 180 K

Total Runtime: 1398.43 seconds

Best Verlet Algorithm: Velocity-Verlet (Adaptive)

Best Time Step: 5.00×10^{-16} s

Reason: Lowest average potential energy (-1.29×10^{-20} J) and minimal energy drift (5.21×10^{-23} J) during preliminary simulation.

