Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2809e-10 m

Melting Point: 185 K

Boiling Point: 200 K

Total Runtime: 264.22 seconds

Best Verlet Algorithm: Velocity-Verlet (Adaptive)

Best Time Step: 1.00e-15 s

Reason: Lowest average potential energy (-1.31e-20 J) and minimal energy drift (6.16e-24 J) during preliminary simulation.