Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2756e-10 m

Melting Point: 185 K

Boiling Point: 190 K

Total Runtime: 1104.42 seconds

Best Verlet Algorithm: Leapfrog Verlet (Adaptive)

Best Time Step: 5.00e-16 s

Reason: Lowest average potential energy (-1.21e-20 J) and minimal energy drift (5.97e-23 J) during preliminary simulation.