Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2756e-10 m

Melting Point: 155 K

Boiling Point: 165 K

Total Runtime: 1220.30 seconds

Best Verlet Algorithm: Leapfrog Verlet (Adaptive)

Best Time Step: 1.00e-14 s

Reason: Lowest average potential energy (-1.30e-20 J) and minimal energy drift (2.88e-23 J) during preliminary simulation.