Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2756e-10 m

Melting Point: 170 K

Boiling Point: 200 K

Total Runtime: 909.62 seconds

Best Verlet Algorithm: Velocity-Verlet (Adaptive)

Best Time Step: 5.00e-15 s

Reason: Lowest average potential energy (-1.27e-20 J) and minimal energy drift (6.46e-23 J) during preliminary simulation.