Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2756e-10 m

Melting Point: 75 K

Boiling Point: 190 K

Total Runtime: 2409.45 seconds

Best Verlet Algorithm: Velocity-Verlet (Adaptive)

Best Time Step: 5.00e-15 s

Reason: Lowest average potential energy (-1.21e-20 J) and minimal energy drift (2.51e-23 J) during preliminary simulation.