Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2753e-10 m

Melting Point: 110 K

Boiling Point: 185 K

Total Runtime: 2726.30 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 (3.48e-23 J) during preliminary simulation.