Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2823e-10 m

Melting Point: 120 K

Boiling Point: 165 K

Total Runtime: 4871.72 seconds

Best Verlet Algorithm: Velocity-Verlet (Adaptive)

Best Time Step: 1.00e-15 s

Reason: Lowest average potential energy (-1.29e-20 J) and minimal energy drift (6.22e-24 J) during preliminary simulation.