Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2823e-10 m

Melting Point: 120 K

Boiling Point: 195 K

Total Runtime: 1226.64 seconds

Best Verlet Algorithm: Leapfrog Verlet (Adaptive)

Best Time Step: 5.00e-16 s

Reason: Lowest average potential energy (-1.29e-20 J) and minimal energy drift
(2.26e-24 J) during preliminary simulation.