Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2823e-10 m

Melting Point: 120 K

Boiling Point: 155 K

Total Runtime: 3998.09 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 (8.96e-24 J) during preliminary simulation.