Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2776e-10 m

Melting Point: 170 K

Boiling Point: 190 K

Total Runtime: 829.11 seconds

Best Verlet Algorithm: Leapfrog Verlet (Adaptive)

Best Time Step: 1.00e-16 s

Reason: Lowest average potential energy (-1.27e-20 J) and minimal energy drift (7.62e-23 J) during preliminary simulation.