Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2756e-10 m

Melting Point: 180 K

Boiling Point: 195 K

Total Runtime: 633.73 seconds

Best Verlet Algorithm: Standard Verlet (Adaptive)

Best Time Step: 1.00e-15 s

Reason: Lowest average potential energy (-1.29e-20 J) and minimal energy drift (2.00e-22 J) during preliminary simulation.