Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2742e-10 m

Melting Point: 120 K

Boiling Point: 145 K

Total Runtime: 3768.11 seconds

Best Verlet Algorithm: Velocity-Verlet (Adaptive)

Best Time Step: 5.00e-16 s

Reason: Lowest average potential energy (-1.41e-18 J) and minimal energy drift (7.74e-24 J) during preliminary simulation.