Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2823e-10 m

Melting Point: 95 K

Boiling Point: 145 K

Total Runtime: 95.69 seconds

Best Verlet Algorithm: Velocity-Verlet (Adaptive)

Best Time Step: 1.00e-14 s

Reason: Lowest average potential energy (-1.31e-20 J) and minimal energy drift (2.67e-25 J) during preliminary simulation.