Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2823e-10 m

Melting Point: 80 K

Boiling Point: 125 K

Total Runtime: 1627.04 seconds

Best Verlet Algorithm: Velocity-Verlet (Adaptive)

Best Time Step: 1.00e-15 s

Reason: Lowest average potential energy (-1.22e-20 J) and minimal energy drift (4.85e-23 J) during preliminary simulation.