Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2809e-10 m

Melting Point: 130 K

Boiling Point: 155 K

Total Runtime: 63.04 seconds

Best Verlet Algorithm: Velocity-Verlet (Adaptive)

Best Time Step: 1.00e-15 s

Reason: Lowest average potential energy (-1.19e-20 J) and minimal energy drift (8.25e-25 J) during preliminary simulation.