Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2756e-10 m

Melting Point: 40 K

Boiling Point: 145 K

Total Runtime: 552.09 seconds

Best Verlet Algorithm: Standard Verlet (Adaptive)

Best Time Step: 1.00e-15 s

Reason: Lowest average potential energy (-1.30e-20 J) and minimal energy drift (2.09e-22 J) during preliminary simulation.