Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2727e-10 m

Melting Point: 75 K

Boiling Point: 170 K

Total Runtime: 1322.95 seconds

Best Verlet Algorithm: Standard Verlet (Adaptive)

Best Time Step: 5.00e-17 s

Reason: Lowest average potential energy (-1.41e-18 J) and minimal energy drift (3.50e-24 J) during preliminary simulation.