Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2756e-10 m

Melting Point: 60 K

Boiling Point: 145 K

Total Runtime: 1350.99 seconds

Best Verlet Algorithm: Leapfrog Verlet (Adaptive)

Best Time Step: 1.00e-15 s

Reason: Lowest average potential energy (-1.21e-20 J) and minimal energy drift (2.32e-23 J) during preliminary simulation.