Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2776e-10 m

Melting Point: 190 K

Boiling Point: 200 K

Total Runtime: 30.08 seconds

Best Verlet Algorithm: Leapfrog Verlet (Adaptive)

Best Time Step: 1.00e-15 s

Reason: Lowest average potential energy (-1.32e-20 J) and minimal energy drift (1.43e-24 J) during preliminary simulation.