Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2826e-10 m

Melting Point: 180 K

Boiling Point: 190 K

Total Runtime: 967.43 seconds

Best Verlet Algorithm: Velocity-Verlet (Adaptive)

Best Time Step: 1.00e-15 s

Reason: Lowest average potential energy (-1.23e-20 J) and minimal energy drift (2.23e-23 J) during preliminary simulation.