Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2742e-10 m

Melting Point: 165 K

Boiling Point: 170 K

Total Runtime: 4656.00 seconds

Best Verlet Algorithm: Velocity-Verlet (Adaptive)

Best Time Step: 1.00e-16 s

Reason: Lowest average potential energy (-1.41e-18 J) and minimal energy drift (3.77e-24 J) during preliminary simulation.