Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2727e-10 m

Melting Point: 55 K

Boiling Point: 165 K

Total Runtime: 564.38 seconds

Best Verlet Algorithm: Standard Verlet (Adaptive)

Best Time Step: 1.00e-16 s

Reason: Lowest average potential energy (-1.41e-18 J) and minimal energy drift (3.79e-23 J) during preliminary simulation.