Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2742e-10 m

Melting Point: 35 K

Boiling Point: 150 K

Total Runtime: 4871.92 seconds

Best Verlet Algorithm: Velocity-Verlet (Adaptive)

Best Time Step: 1.00e-15 s

Reason: Lowest average potential energy (-1.41e-18 J) and minimal energy drift (1.10e-23 J) during preliminary simulation.