

Molecular Dynamics Simulation Report

Optimized Lattice Parameter: 5.2756×10^{-10} m

Melting Point: 170 K

Boiling Point: 200 K

Total Runtime: 1316.82 seconds

Best Verlet Algorithm: Standard Verlet (Adaptive)

Best Time Step: 5.00×10^{-15} s

Reason: Lowest average potential energy (-1.27×10^{-20} J) and minimal energy drift (3.51×10^{-23} J) during preliminary simulation.

