An Integrated Molecular–Thermodynamic Framework for Analyzing Nanobubbles in Supersaturated Liquids

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Electronic Supplementary Information

Forcefield Verification Using Nanobubble Density Analysis

To verify the compatibility of the selected forcefields for hydrogen and water, we compared the nanobubble density obtained from MD simulations ($n_{gB}M_g/V_{gB}$) with the hydrogen density calculated from NIST data, using the corresponding bubble pressure and temperature. Figure S-1 illustrates the comparison for the systems S4 and L5. The densities from MD simulations align closely with the NIST estimates, falling along the 45-degree line. These results confirm that the chosen forcefields accurately model the water-hydrogen interactions.

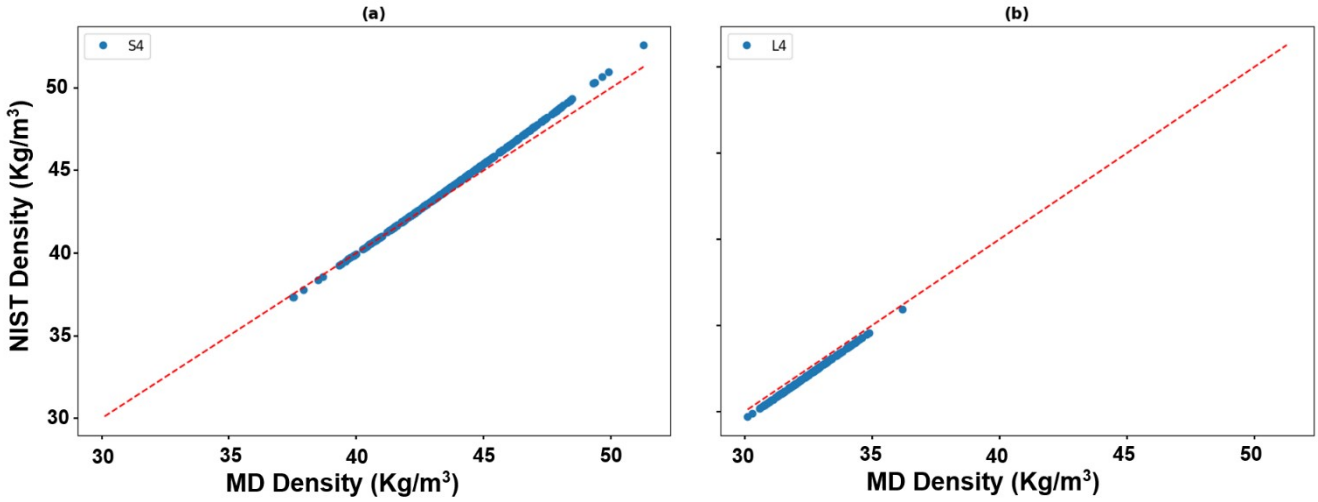

Figure S-1. Comparison of the hydrogen bubble mass density in water from MD results with NIST data for system (a) S4 and (b) L4.