Open-boundary molecular dynamics of ultrasound using supramolecular water models

Supplementary material

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1 Equilibrium mass density profile

Fig. S1 shows the equilibrium density profile through the open direction for the DPD 4-to-1 model in OBMD. The fluctuations in the region of interest (ROI) are consistent with the equilibrium density fluctuations of a grand canonical ensemble.

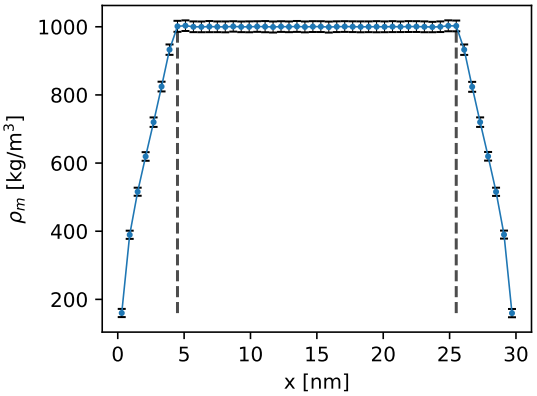

Figure S1: Equilibrium mass density profile for the DPD 4-to-1 water model in OBMD. The dashed lines represent the borders of the ROI. The errors are the standard deviations of the binned densities.

2 Cycle-averaged density signals for ultrasound waves

In Fig. S2, we show the computed density signals for ultrasound of different frequencies for all models used. This data was used to determine the phase velocities v_p and attenuation coefficients α in Table IV of the main text.

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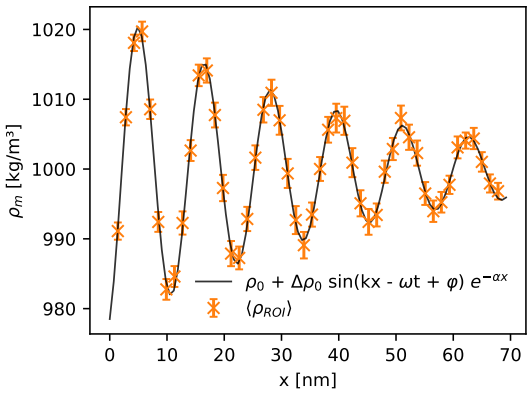
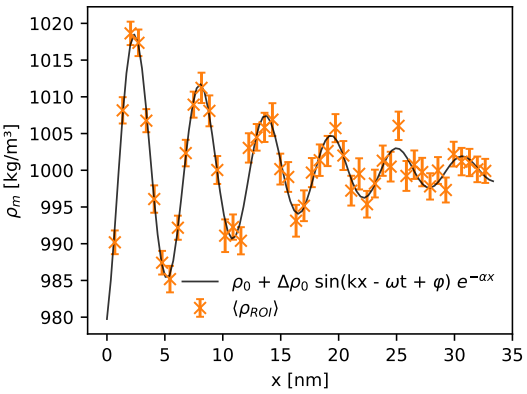
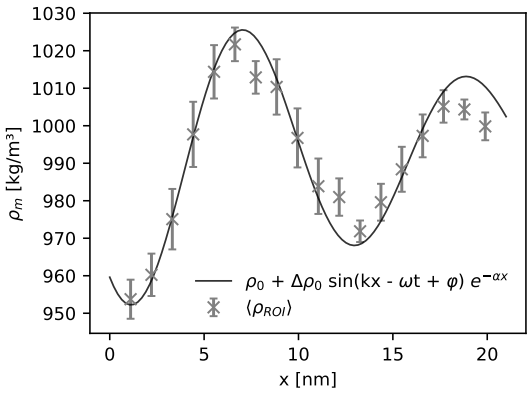


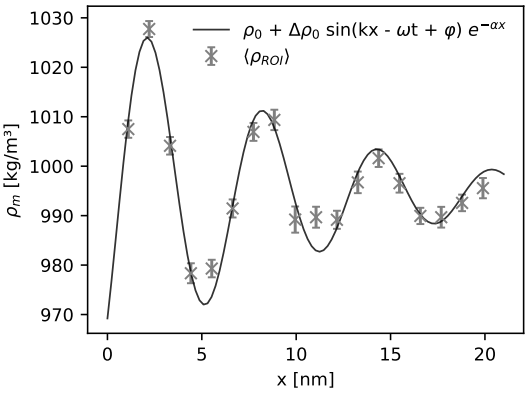
(a) DPD 4-to-1, $\nu = 0.13$ THz



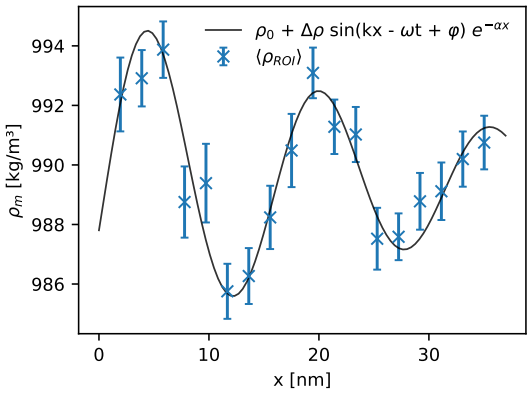
(b) DPD 4-to-1, $\nu = 0.27$ THz



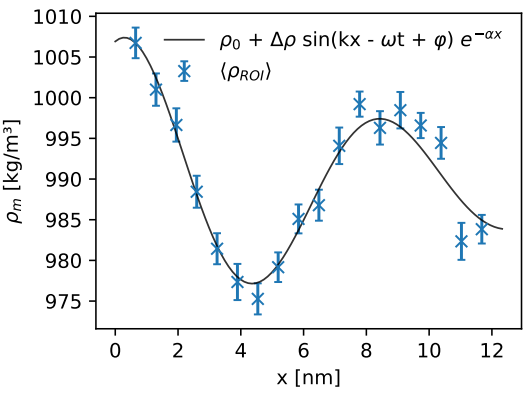
(c) DPD 8-to-1, $\nu = 0.13$ THz



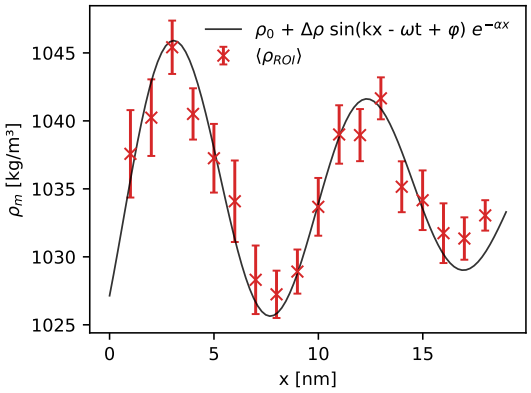
(d) DPD 8-to-1, $\nu = 0.27$ THz



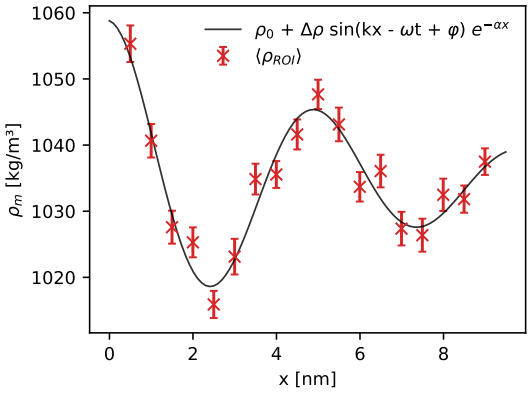
(e) MDPD 3-to-1, $\nu = 0.13$ THz



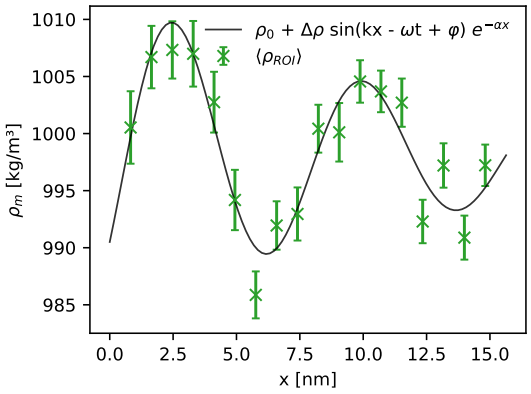
(f) MDPD 3-to-1, $\nu = 0.27$ THz



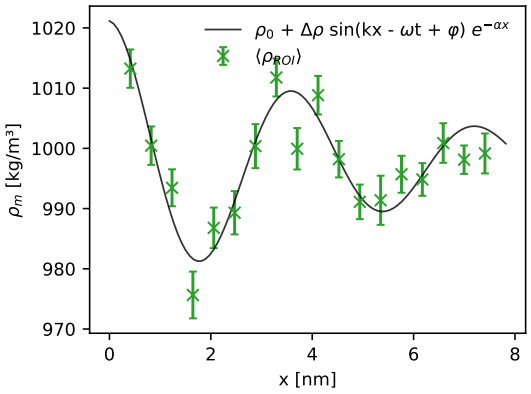
(g) MDPD 4-to-1, $\nu = 0.13$ THz



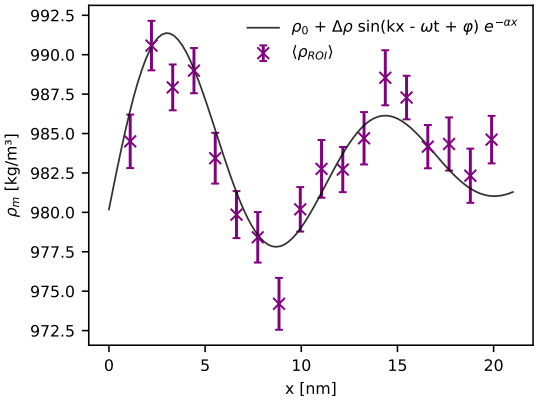
(h) MDPD 4-to-1, $\nu = 0.27$ THz



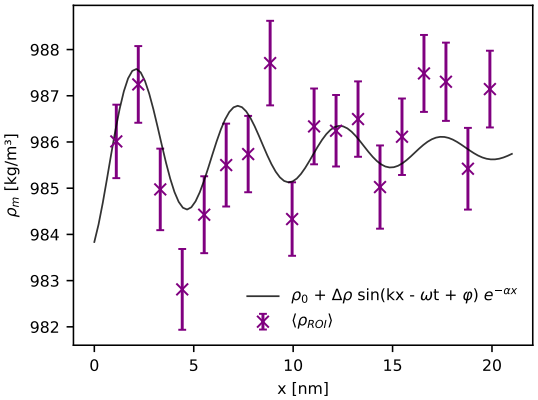
(i) MDPD 8-to-1, $\nu = 0.13$ THz



(j) MDPD 8-to-1, $\nu = 0.27$ THz



(k) Martini 3, $\nu = 0.13$ THz



(l) Martini 3, $\nu = 0.27$ THz

Figure S2: Computed density signals for ultrasound waves of 0.13 THz (left) and 0.27 THz (right) with standard errors. Orange, gray, blue, red, green, and violet data points correspond to DPD 4-to-1, 8-to-1, MDPD 3-to-1, 4-to-1, 8-to-1, and Martini 3 water model, respectively. The black lines are the fitted solutions of the traveling wave equation.

3 Bulk viscosity

Fig. S3 shows how the cumulative integral converges to the bulk viscosity value as the upper limit τ of Eq. (33) increases.

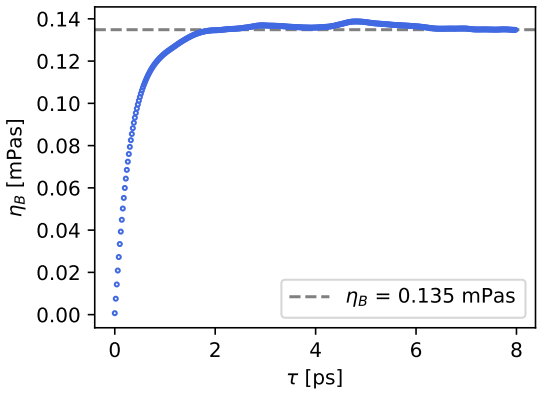


Figure S3: Bulk viscosity for the DPD 4-to-1 model. τ is the upper limit of the integral in Eq. (33). The integral converges to $\eta_B \approx 0.135$ mPas.