

Supporting Information (SI)

Nanobubble size controls gas hydrate nucleation in supercooled water

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I. Equilibration Simulations. The equilibrium simulations are performed in an isothermal-isobaric ensemble (NPT) at 300 K and 10 MPa. Initially, gas and water molecules are randomly placed in the simulation box. Figure S1 shows the energy, temperature, and pressure of the system during the equilibrium simulations. The energy, temperature, and pressure are stabilized during the equilibrium runs.

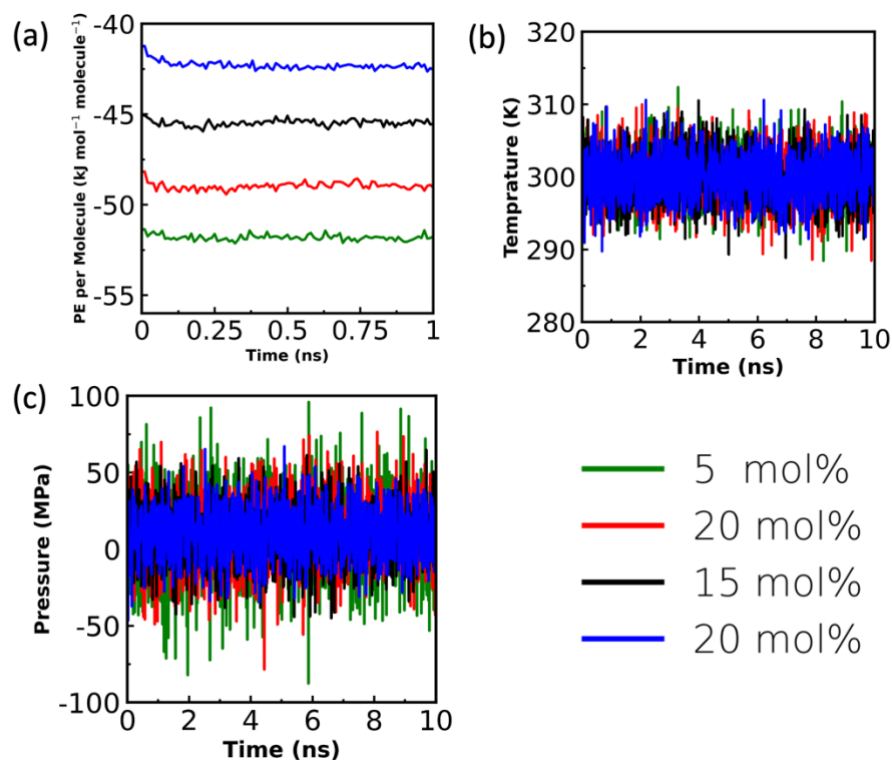


Figure S1: Equilibration simulations. (a), (b), and (c) correspond to energy, temperature and pressure of the system. The data are shown for four cases, each for a specific gas concentration

II. Production Simulations. The production simulations are performed in an isothermal-isobaric ensemble (NPT) at 240 K and 50 MPa. The last configuration of the equilibration run is used as the initial structure of the production run. Figure S2 shows the energy, temperature, and pressure of the system during the equilibrium simulations. The energy gradually decreases as the system undergoes nucleation and growth. The temperature and pressure remain stable during the production runs.

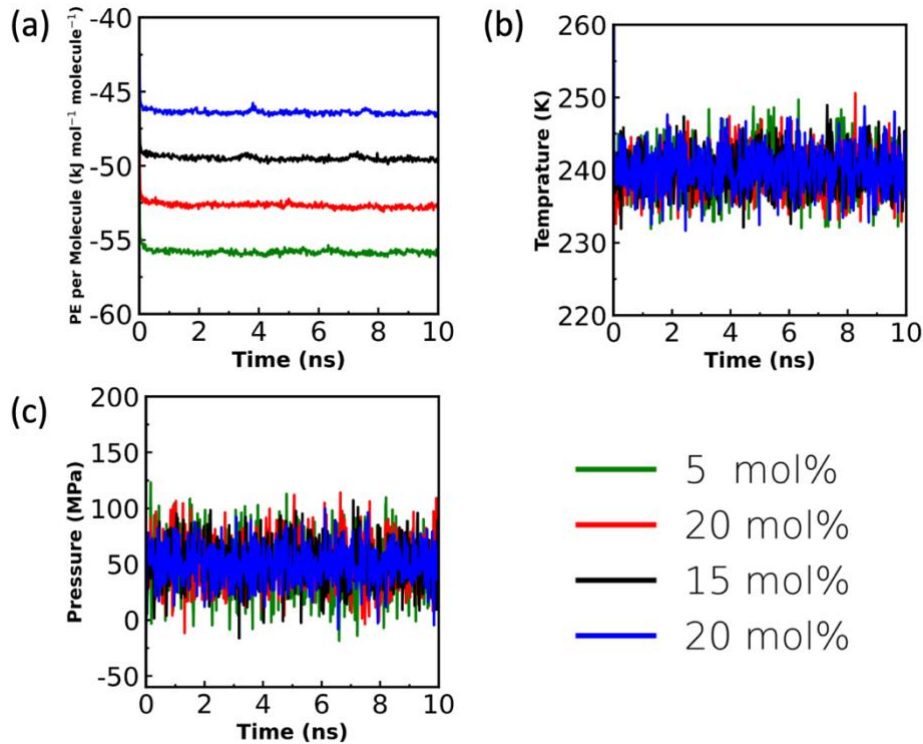


Figure S2: Production simulations. (a), (b), and (c) correspond to energy, temperature and pressure of the system. The data are shown for four cases, each for a specific gas concentration

III. Time evolution of a bubble: We track the largest bubble in the production trajectories. The size of the largest bubble is plotted as a function of time in Figure S3. We observe a size-dependent dissociation of the bubble during the production run.

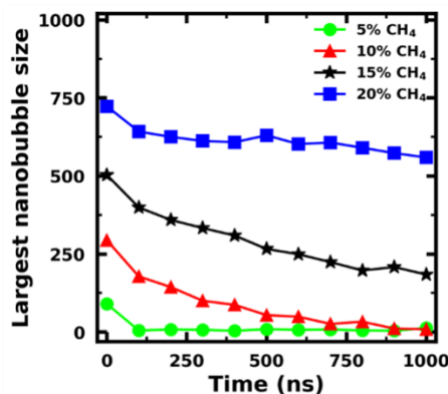


Figure S3: Largest nanobubble size is plotted as a function of time during the production cycle.