

Article

Structural Stabilization Mechanisms and Energy Distribution Patterns of Nanobubbles with Different Sizes

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Abstract

Traditional macroscopic interfacial theory cannot fully explain the anomalous stability of nanobubbles, which limits their use in micro/nano interfacial engineering. In this study, molecular dynamics simulations were used to systematically investigate the evolution of oxygen nanobubbles with diameters of 3, 5, and 8 nm in water. The results show a clear size effect in bubble structural evolution: the 3 nm bubble had the largest motion radius, about 3.5 nm, which was 40% and 133% larger than those of the 5 and 8 nm bubbles, respectively. At the nanoscale, surface tension still provides a basic constraint, but its value is lower than the classical theoretical prediction, with a deviation of 35.7% for the 3 nm bubble, indicating that it is not the sole dominant stabilizing force. Water molecules at the gas–liquid interface experienced a net force of 371.92–421.56 pN, with 60–65% directed toward the bubble interior, forming an asymmetric force field that co-operates with surface tension to maintain bubble stability. This force field further drives directional polarization of water molecules and induces a dense hydrogen-bond network: stronger charge parameters correspond to denser hydrogen bonding, with the peak net charge of Charge4 being 37.5 times that of Charge1 and the hydrogen-bond number being 11.6 times that of Charge2. The dense hydrogen-bond network is quantitatively associated with restricted interfacial water mobility. The interfacial potential energy decreases, with an 8 nm bubble showing a reduction of 0.31 kcal/mol, and the U–T coupling energy exhibits a clear interfacial peak of 36–66 kcal/mol. Further analysis shows that the apparent diffusion coefficient decreases nearly exponentially with the maximum hydrogen-bond number, and the water MSD decreases markedly as hydrogen bonding increases, with the MSD of Charge1 being 1303 times that of Charge4. These results indicate that enhanced interfacial electrostatic force, densification of the hydrogen-bond network, and restricted interfacial water mobility jointly increase structural constraints at the gas–liquid interface and suggest a possible increase in gas-transfer resistance across the interface. This study clarifies, at the molecular scale, a physical picture in which surface tension, electrostatic force, hydrogen-bond densification, energy stabilization, and restricted mobility jointly maintain nanobubble stability.

Keywords: nanobubbles; molecular dynamics; hydrogen bond network; interfacial stability; micro-nano technology



Academic Editor: Weizhong Dai

Received: 5 June 2026

Revised: 29 June 2026

Accepted: 9 July 2026

Published: 12 July 2026

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1. Introduction

Bubbles are typical interfacial structures that exist widely in materials, energy, biology, medicine, and many other fields, where they play important roles in gas transport, liquid-phase mass transfer, and interfacial reactions [1]. Traditional studies have mainly focused on millimeter-scale bubbles, for which relatively complete theories of dynamic behavior and interfacial properties have been established. With the development of interface science toward smaller length scales, small bubbles at the micrometer scale and below have shown unique physicochemical properties and strong application potential in micromixing, surface cleaning, and targeted transport [2]. Compared with large bubbles, small bubbles have larger specific surface area, higher interfacial stability, and superior mass-transfer efficiency [3]. They can enter smaller structural spaces and act on local interfaces, which gives them advantages in precision scenarios such as chip cleaning and cell manipulation [4]. From an application perspective, nanobubble stability directly determines gas retention time, oxygen-transfer efficiency, and the duration of interfacial reactions, and thus affects the generation of local reactive species in water treatment, groundwater remediation, catalytic oxidation, and biomedical microbubble systems. Recent work by Ge et al. further showed that entrapped bubbles can act as both O₂ sinks and sources during surface-water and groundwater interactions and participate in reactive oxygen species production, indicating that nanobubble stability is closely related to oxygen transport and reaction activity in environmental processes [5]. Therefore, nanobubble stability is not only an interfacial physics issue but also a key factor in oxygen-transfer efficiency and environmental reactions.

Small-bubble research has continued for several decades, but most studies have still focused on bubbles larger than 1 micrometer [6], mainly using high-speed photography and optical microscopy to examine bubble generation, motion, and rupture [7]. Traditional bubble theory generally explains bubble stability using Laplace pressure and interfacial tension, assuming that internal pressure is inversely related to bubble radius and that surface tension provides the main morphological constraint [8,9]. However, nanobubbles can remain stable in solution for several days and retain stable spherical morphology at solid–liquid interfaces, with dissolution rates and apparent contact angles that deviate from classical theoretical predictions [10–12]. These observations indicate that nanobubble stability cannot be explained only by Laplace pressure or a single surface-tension term, but should be considered together with interfacial charge, gas diffusion, liquid-phase environment, and molecular-scale interfacial structure [13,14].

Direct evidence for nanobubbles was long limited by the spatial resolution of traditional characterization methods [15]. In 2001, atomic force microscopy (AFM) first clearly observed nanobubbles at solid–liquid interfaces [16], promoting systematic research in this field. Since then, AFM, light scattering, and confocal microscopy have gradually revealed the size distribution, interfacial structure, and stability mechanisms of nanobubbles [17]. Compared with micrometer-scale bubbles, nanobubble stability is affected not only by surface tension and gas diffusion but also by the surrounding molecular environment [18]. Nevertheless, experimental characterization mainly reflects interfacial morphology and population-scale features and is difficult to use for directly obtaining internal pressure, interfacial molecular orientation, and local energy changes. Therefore, molecular-scale analysis of boundary evolution, internal structure, and energy distribution is essential for understanding nanobubble stability.

Because the microscopic composition and structure of bubbles, including interfacial density distribution, internal energy state, and molecular arrangement, directly affect stability, dissolution behavior, and dynamic evolution [19], methods with molecular resolution are needed to analyze internal structure and evolution. In recent years, molecular

dynamics (MD) simulation has made it possible to describe bubble formation, evolution, and interfacial changes at atomic or molecular resolution and has been widely used for liquid–gas interfaces and bubble dynamics. MD studies have shown pronounced temperature and density fluctuations at nanobubble gas–liquid interfaces, and the apparent contact angle changes dynamically with interfacial molecular arrangement, which extends beyond the applicability of traditional macroscopic contact-angle models [20]. At the nanoscale, bubble stability is controlled not only by classical size effects but also by interfacial water orientation and gas transport behavior [21]. Recent large-scale atomistic and MD studies also show that the stability of oxygen or hydrogen nanobubbles is closely related to bubble construction, internal pressure, diffuse interfacial structure, gas transport, and external perturbations, indicating the need to consider interfacial mechanics and mass transfer together at the molecular scale [22,23].

Existing studies have mainly focused on overall bubble behavior and external interfacial changes, whereas the coupling among internal structure, density distribution, and microscopic energy evolution remains insufficiently discussed [24]. Therefore, this study uses LAMMPS (29 August 2024) molecular dynamics simulations to construct single oxygen nanobubbles with diameters of 3, 5, and 8 nm and examine their natural evolution under constant-temperature and constant-pressure conditions. Boundary profiles, density distributions, pressure and apparent surface tension, interfacial force, charge distribution, hydrogen-bond structure, and water-molecule mobility are jointly analyzed to reveal the multi-factor synergistic mechanism of nanobubble stability under the particle-size effect.

2. Materials and Methods

2.1. Modeling Method of Oxygen Nanobubbles in Aqueous Phase

Initial molecular structures of water and oxygen were constructed in Materials Studio (2023, BIOVIA, San Diego, CA, USA) and then imported into LAMMPS (29 August 2024, Sandia National Laboratories, Albuquerque, NM, USA) for nanobubble simulations. The simulation workflow included energy minimization, NPT pre-equilibration, and comparative NVT/NPT simulations. After the systems reached a quasi-stable state, evaluated from the time evolution of density distribution, bubble radius, pressure distribution, and system energy, bubble structure and interfacial properties were analyzed. Because the NPT ensemble allows the simulation box volume to respond to pressure, it more reasonably reflects the natural evolution of nanobubbles in the liquid phase. As shown in Figure S1, the bubble motion range under NPT conditions was larger than that under NVT conditions. Therefore, all analyses of bubble stability, structural evolution, and interfacial properties in this study are based on NPT trajectories, while NVT results are used only as an auxiliary comparison. Detailed simulation parameters and the NVT/NPT comparison are provided in Text S1, and the modeling and calculation workflow is shown in Figure 1.

2.1.1. Atomic Model Construction of Water and Oxygen Molecules

Three cubic water boxes were constructed by MD simulation and filled with different numbers of water molecules according to the target density (Figure S2). Water molecules were described by the classical SPC/E model [25,26], which is widely used in aqueous interfacial simulations and offers a balance between structural description and computational efficiency, making it suitable for consistent comparison among multiple bubble sizes and charge conditions. Oxygen was modeled as a diatomic all-atom molecule with an O=O bond length of 1.207 Å and a bond force constant of 500 kcal/mol/Å² to maintain molecular structural stability [27]. Non-bonded interactions between oxygen and water molecules were described by Lennard-Jones potentials, and cross parameters were calculated using the Lorentz–Berthelot mixing rule. The specific parameters are listed in Table S1.

2.1.2. Construction of Nanobubbles Based on the Cavity Method

Nanobubbles were constructed using the cavity method. Spherical water regions with radii of 1.5, 2.5, and 4.0 nm were removed from the centers of the simulation boxes to generate initial cavities with target diameters of 3, 5, and 8 nm, respectively. Oxygen molecules were then randomly inserted into the cavities. The water box size was larger than the corresponding bubble size, and the liquid buffer distance between the bubble interface and the simulation boundary was greater than the non-bonded interaction cutoff length, reducing direct short-range interactions between the bubble and its periodic images. The initial O₂ mass density was approximately 0.4 g/cm³, corresponding to about 450, 2000, and 6500 oxygen molecules for the 3, 5, and 8 nm systems, respectively (Figure S2), ensuring comparable initial states.

2.2. Calculation Methods for Bubble Internal Pressure and Apparent Surface Tension

Bubble pressure was calculated from the radial pressure distribution obtained from molecular dynamics simulations. Considering the spatial nonuniformity of the gas–liquid interface, local pressure was statistically averaged in radial spherical shells across the bubble core, interfacial region, and external liquid phase, and the internal–external pressure difference ΔP was then obtained. The bubble radius R was determined from the radial density distribution and apparent surface tension. Because the nanobubble interface is diffuse and this value is derived from the simulated pressure difference and instantaneous radius, it is referred to here as the apparent surface tension.

The above conversion is based on the Young–Laplace relationship (de Gennes et al., 2004) [28], which describes the relationship among internal–external pressure difference, bubble radius, and interfacial tension in a macroscopic continuum:

$$P_{\text{in}} - P_{\text{out}} = \frac{2\gamma}{R} \quad (1)$$

Here, P_{in} and P_{out} denote the internal and external pressures of the bubble, respectively, γ is the interfacial tension, and R is the bubble radius. In a macroscopic continuum framework, this relationship indicates that the pressure difference is proportional to interfacial tension and inversely proportional to bubble radius. In this study, the equation is not used as an independent pressure-prediction method; rather, it converts the simulated ΔP and R into an apparent surface tension for comparison with macroscopic theoretical values.

2.3. Calculation Methods for Bubble Density Distribution and Inner/Outer Radii

The clarity and location of the bubble boundary are important indicators of nanobubble stability. Using the radial distribution function (RDF) and spherical-shell statistics [29], the number-density distribution $\rho_n(r)$ was obtained at different radial positions from the bubble center outward:

$$\rho_n(r) = \frac{1}{4\pi r^2 \Delta r} N(r) \quad (2)$$

where r represents the radial distance, Δr denotes the shell thickness, and $N(r)$ indicates the number of atoms within that shell. The number density can then be converted into mass density:

$$\rho_m(r) = \rho_n(r) \times m \quad (3)$$

The inner and outer radii of the bubble can be determined by analyzing the variation curves of oxygen and water density. The inner radius is identified when the oxygen density sharply decreases by more than 95% from its peak value. In contrast, the outer radius is determined when the water density increases to 90–95% of its bulk uniform value, which is approximately 0.9 g/cm³.

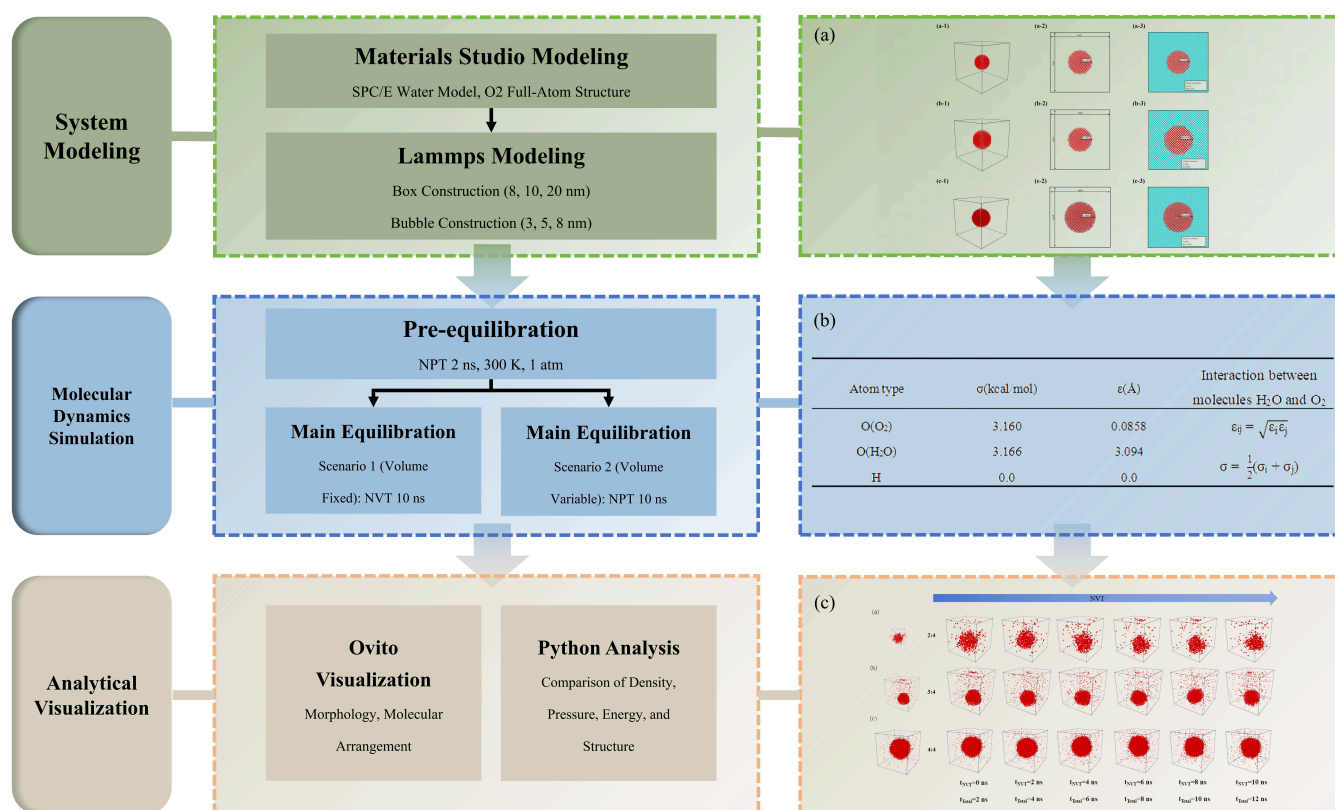


Figure 1. Flowchart of the molecular dynamics simulation procedure for nanobubbles. The right-side panels show three key steps: **(a)** molecular and system modeling, including the SPC/E water model, O₂ molecules, and initial box construction parameters (details in Figure S2); **(b)** force-field parameter determination, including Lennard-Jones interactions and parameters between water and oxygen molecules (details in Table S1); and **(c)** Brownian-motion visualization of red oxygen molecules and blue water molecules forming 3, 5, and 8 nm bubbles (details in Figure S1).

2.4. Energy Distribution Calculation and Structural Stability Evaluation

Bubble stability is directly affected by its internal and interfacial energy distributions. Molecular dynamics simulations were used to calculate the kinetic energy (KE), potential energy (PE), and total energy (U) of the bubbles, and energy variations at different radial positions were analyzed to evaluate bubble stability [20]. In the simulations, KE was obtained from the velocity of each atom in the bubble:

$$KE(r) = \sum_i \frac{1}{2} m_i v_i^2 \quad (4)$$

where m_i is the mass of atom i and v_i is its velocity. Simulations at different time steps and bubble sizes provided the radial KE distribution, showing that KE tends to increase as bubble size increases [30]. PE reflects the strength of intermolecular interactions in and around the bubble and is expressed as:

$$PE(r) = \sum_{ij} \frac{C_{ij}}{r_{ij}} \quad (5)$$

where r_{ij} denotes the distance between the i th and j th atoms, while C_{ij} represents the potential energy parameter. The PE distribution underscores the variation in interaction strength between the interior and exterior regions of the bubble.

The total energy (E) is calculated by adding the KE and PE, using the following formula:

$$U(r) = KE(r) + PE(r) \quad (6)$$

In addition to kinetic and potential energies, this study calculated the U–T coupling energy to compare the relative response of local internal energy to temperature perturbation in different radial regions [31]. The index is calculated as follows:

$$F = U - T \left(\frac{dU}{dT} \right) \quad (7)$$

where U is the local internal energy of the bubble system, T is temperature, and dU/dT was estimated from the slope of internal-energy variation with temperature between adjacent statistical windows. Therefore, U–T coupling energy is mainly used to compare relative response strength among different radial regions and bubble-size systems.

2.5. Calculation Methods for Hydrogen Bond Number and Energy

The hydrogen-bond network is a key factor for maintaining the structural stability of the gas–liquid interface. To quantify hydrogen-bond characteristics, a geometric criterion was used for hydrogen-bond identification. A hydrogen bond was defined when the donor oxygen atom (D) and acceptor oxygen atom (A) distance R_{AD} was less than 0.35 nm and the donor-hydrogen-acceptor angle β_{D-H-A} was less than 30° .

The hydrogen-bond number (N_{HBs}) was calculated using radial-shell statistics [32]. The simulation system was divided into concentric spherical shells with a thickness of 0.1 nm centered at the bubble center, and the average number of hydrogen bonds formed per water molecule in each shell was counted:

$$N_{HBs}(r) = \frac{\sum_{i=1} N_{shell(r)} n_{HB,i}}{N_{H_2O}} \quad (8)$$

where $N_{shell}(r)$ is the total number of hydrogen bonds formed in the shell at radial distance r , $N_{H_2O}(r)$ is the number of water molecules in that shell, and $n_{HB,i}$ is the number of hydrogen bonds associated with the i th water molecule. Hydrogen-bond energy (E_{HBs}) was calculated based on the standard energy value of a single hydrogen bond, $E_{H-B} = -2.82$ kJ/mol. The total hydrogen-bond energy in a shell is expressed as:

$$E_{HBs}(r) = N_{HBs}(r) \times E_{H-B} \quad (9)$$

To determine the average energy per hydrogen bond, one should divide the total energy by the number of hydrogen bonds.

3. Results and Analysis

3.1. Motion Trajectories and Structural Variation Characteristics of Nanobubbles with Different Sizes

Oxygen nanobubbles with diameters of 3 nm, 5 nm, and 8 nm were modeled using LAMMPS software. In these simulations, oxygen molecules from bubbles of different sizes diffused gradually into the system (as shown in Figure S1), highlighting significant morphological differences. Larger bubbles contained more oxygen molecules, which led to increased outward diffusion and a more stable, spherical shape. The curvature of the bubbles effectively illustrated these morphological changes (Figure S2). As the bubble size increased, curvature fluctuations decreased and stabilized over time. The 3 nm bubble exhibited the most pronounced curvature fluctuation, ranging from -59 to 49 nm $^{-1}$, with an irregular surface. In contrast, the 5 nm bubble showed a narrower curvature range

of -12 to 18 nm^{-1} , with smoother surface undulations. The 8 nm bubble had the most concentrated curvature distribution, ranging from -10 to 5 nm^{-1} , and its surface closely resembled an ideal sphere.

As shown in Figure 2a, the bubble motion characteristics varied according to their size, revealing irregular motion with a smaller bubble diameter. For instance, the 3 nm bubble exhibited the widest range of motion, with a radius of approximately 3.5 nm, which is 40% and 133% larger than the 5 nm and 8 nm bubbles, respectively. During this random motion, oxygen molecules gradually diffused outward from the nanobubble, resulting in a decrease in oxygen number density from the center to the edge. This spatial distribution divides the bubble interior into three regions: the gas region (local oxygen number density $\geq 0.95\rho_0$, where ρ_0 is the maximum oxygen number density at the bubble interface before decline), the gas–liquid mixing region ($0.95\rho_0 > \text{local oxygen number density} > 0.05\rho_0$), and the liquid region (local oxygen number density $\leq 0.05\rho_0$). Figure 2b illustrates the temporal evolution of bubble radii for the three sizes. Between 0 and 2 ns, the inner radii of the bubbles increased to 2.05 nm, 3.72 nm, and 5.1 nm, with growth rates of 36.67%, 48.8%, and 27.5%, respectively. After 2 ns, both inner and outer radii gradually decreased for all sizes. To better understand the impact of bubble size on spatial radii, we calculated the ratios I_{outer} (outer radius to initial radius) and $I_{\text{transition}}$ (transition radius to initial radius). Our findings revealed that both I_{outer} and $I_{\text{transition}}$ decreased as bubble size increased. The 3 nm bubble had the highest values: $I_{\text{outer}} = 1.82$ and $I_{\text{transition}} = 0.53$, which were 12% and 8% higher than those of the 5 nm bubble, and 25% and 24% higher than those of the 8 nm bubble (as detailed in Supplementary Table S2).

Figure 2c,d systematically analyzes radial density distributions, illustrating the evolution of interfacial structures in nanobubbles of different sizes. As the radial distance extends from the gas region to the outer liquid region, the average oxygen density dropped sharply from 0.31–0.82 g/cm³ to nearly zero. Meanwhile, the average water density increased from nearly zero to about 0.9 g/cm³. In the gas region, the 8 nm bubble achieved an average density of 0.82 g/cm³, which was 50% and 161% higher than those of the 3 nm and 5 nm bubbles, respectively. Furthermore, the density fluctuation range in this region increased with bubble size; the 8 nm bubble showed a fluctuation value of 1.23 g/cm³, approximately 73% and 62% higher than the 3 nm and 5 nm bubbles, respectively. In the gas–liquid mixing region, the average oxygen density significantly decayed to varying degrees, with the 8 nm bubble experiencing a reduction of 0.63 g/cm³, which was approximately 54% and 162% greater than the decreases observed in the 3 nm and 5 nm bubbles, respectively.

3.2. Pressure Distribution Patterns Inside and at the Interface of Bubbles

Figure 3a–c shows the radial pressure distribution within a nanobubble. As the radial distance extends from the bubble's center to the outer liquid region, the oxygen molecule pressure and the total system pressure decreased from 250–470 atm in the gas region to about 70 atm and 90 atm in the liquid region, respectively. This reduction clearly indicated a typical high-to-low pressure profile. Notably, pressure distribution patterns for bubbles of different sizes exhibited minimal variation over time (see Supplementary Figure S4). In the gas region, the pressure curves for oxygen molecules and the total system completely overlapped, with average pressure decreasing as bubble size increased. The 3 nm bubble revealed the highest average pressure (≈ 470 atm), which was 30.6% and 88.0% higher than that of the 5 nm and 8 nm bubbles, respectively. In the gas–liquid mixing region, the oxygen pressure dropped rapidly, decreasing to 360 atm in the 3 nm bubble, which represented 28.6% and 125% greater than those in the 5 nm and 8 nm bubbles. Conversely, the total system pressure declined more moderately in this region, with all three sizes showing a drop of 200 atm. Within this zone, the water molecule pressure first declined and then

increased, with the 3 nm bubble reaching the lowest negative-pressure trough (≈ -550 atm), about 19.6% and 48.6% lower than that of the 5 nm and 8 nm bubbles, respectively. In the liquid region, the total pressure stabilized around 90 atm; the water molecule pressure rose and remained near 20 atm, while the oxygen molecule pressure decayed to approximately 60 atm.

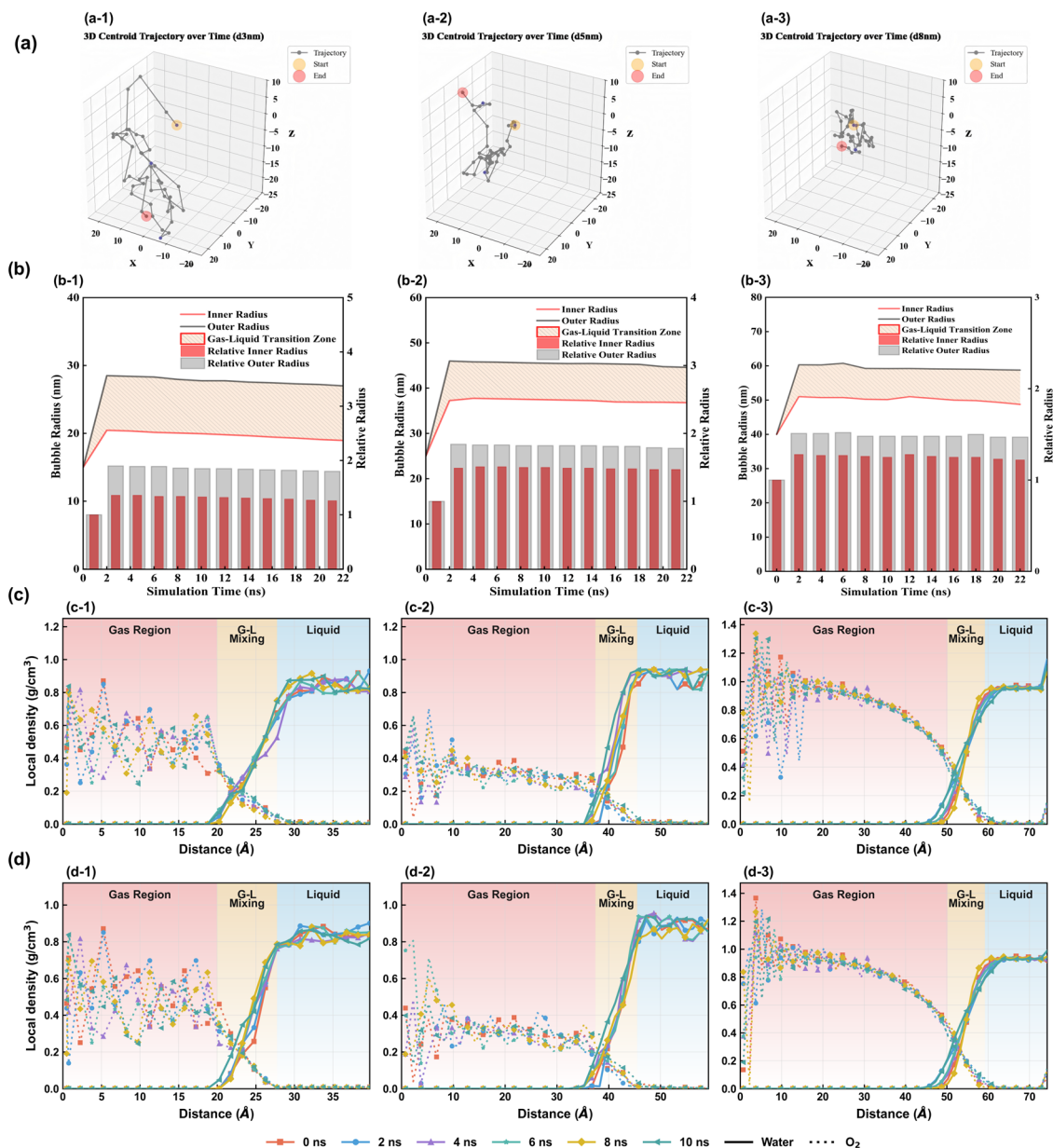


Figure 2. Multi-scale dynamic behavior of nanobubbles with different sizes. (a-1–a-3) Centroid trajectories of 3, 5, and 8 nm bubbles, respectively, constructed from 40 instantaneous centroid positions sampled at equal time intervals from 0 to 20 ns. The black curve represents the centroid trajectory, the yellow point denotes the initial centroid position, and the red point denotes the final centroid position. (b-1–b-3) Radius evolution and interfacial characteristics of 3, 5, and 8 nm bubbles. The left axis shows the inner radius (red curve) and outer radius (black curve), and the gray area between them represents gas–liquid interface thickness. The right axis shows the ratios relative to the initial size: red bars represent transition radius/initial radius, and gray bars represent outer radius/initial radius. (c-1–c-3) and (d-1–d-3) show temporal radial density distributions from spherical-shell statistics under NVT and NPT ensembles, respectively, for 3, 5, and 8 nm bubbles from left to right.

Figures 3d and S5 show that, within 0–10 ns, the theoretical pressure differences for the 3, 5, and 8 nm bubbles were 440.98–471.48, 338.76–377.52, and 255.04–276.60 atm, respectively, which were 18.2%, 25.9%, and 29.3% higher than the simulated pressure differences. The theoretical surface tensions were 55.12–58.94, 59.28–65.10, and 64.65–66.61 mN/m, respectively, which were 35.7%, 27.7%, and 23.5% higher than the simulated surface tensions. As the simulation time increased from 0 to 10 ns, pressure difference and surface tension increased overall for all bubble sizes. At 10 ns, the surface tension of the 8 nm bubble was about 51 mN/m, 21.4% and 8.5% higher than those of the 3 and 5 nm bubbles, whereas its pressure difference was about 215 atm, 46.4% and 27.9% lower than those of the 3 and 5 nm bubbles. Recent molecular dynamics studies of bulk nanobubbles have also indicated that gas–liquid interfacial layers, hydration layers, interfacial thickness, curvature correction, and molecular arrangement can make nanoscale apparent surface tension deviate from macroscopic theoretical values [22,23,33]. This is consistent with treating the simulated surface tension here as an apparent interfacial mechanical quantity. The difference indicates that Young–Laplace theory overestimates nanoscale pressure difference and surface tension because the nanobubble interface is not a sharp, zero-thickness ideal boundary. Instead, the transition region is jointly formed by oxygen and water molecules, and pressure and density vary continuously along the radial direction. Even so, under the same calculation protocol, the simulated surface tension increases with bubble size and can still reflect relative interfacial constraint strength among different bubble sizes.

Over the 0–10 ns interval, the bubble's surface tension and internal pressure difference increased. By 10 ns, the pressure difference rose to 215–401 atm, marking an approximate 9–11% increase from the baseline at 0 ns. Similarly, the surface tension increased to 42–51 mN/m, reflecting a 3–5% increase from the initial value at 0 ns. As the bubble expanded, the surface tension continued growing, while the pressure difference decreased. For example, the pressure difference for the 8 nm bubble was 215 atm, which was 27.9% and 46.4% lower than that of the 5 nm and 3 nm bubbles, respectively. In contrast, its surface tension of 51 mN/m was 8.5% and 21.4% higher than that of the 5 nm and 3 nm bubbles, respectively.

3.3. Energy Distribution Characteristics Inside and at the Interface of Bubbles

Figure 4 shows the energy distribution characteristics inside and at the interface of the bubbles. As shown in Figure 4a, under different simulation times, the kinetic energies of oxygen and water molecules show clear regional differences along the radial direction. In the bubble core, oxygen molecule kinetic energy remains high, whereas water molecule kinetic energy is close to 0 kcal/mol. The average oxygen kinetic energy in the 8 nm bubble core is 0.62 kcal/mol, about 9.9% and 3.3% higher than those in the 3 and 5 nm bubbles, respectively. After entering the gas–liquid transition zone, oxygen kinetic energy gradually decreases and water kinetic energy rapidly increases. The 8 nm bubble shows the largest increase in water kinetic energy, about 0.508 kcal/mol, 0.4% and 3.2% higher than those of the 3 and 5 nm bubbles. In the liquid region, oxygen kinetic energy approaches 0 kcal/mol, and water kinetic energy stabilizes near 0.648 kcal/mol, about 5.6% higher than that of the 3 nm bubble.

As shown in Figure 4b, under different simulation times, the system potential energy first remains stable and then decreases with increasing radial distance, changing from -0.81 to -0.32 kcal/mol in the bubble core to -0.30 to -0.27 kcal/mol in the liquid region. In the bubble core, the absolute average potential energy of the 8 nm bubble is 0.80 kcal/mol, 56.9% and 110.5% higher than those of the 3 and 5 nm bubbles, respectively. After entering the gas–liquid transition zone, the 8 nm bubble exhibits the largest potential-

energy decrease of 0.31 kcal/mol, about 11.1% and 15.4% greater than those of the 3 and 5 nm bubbles.

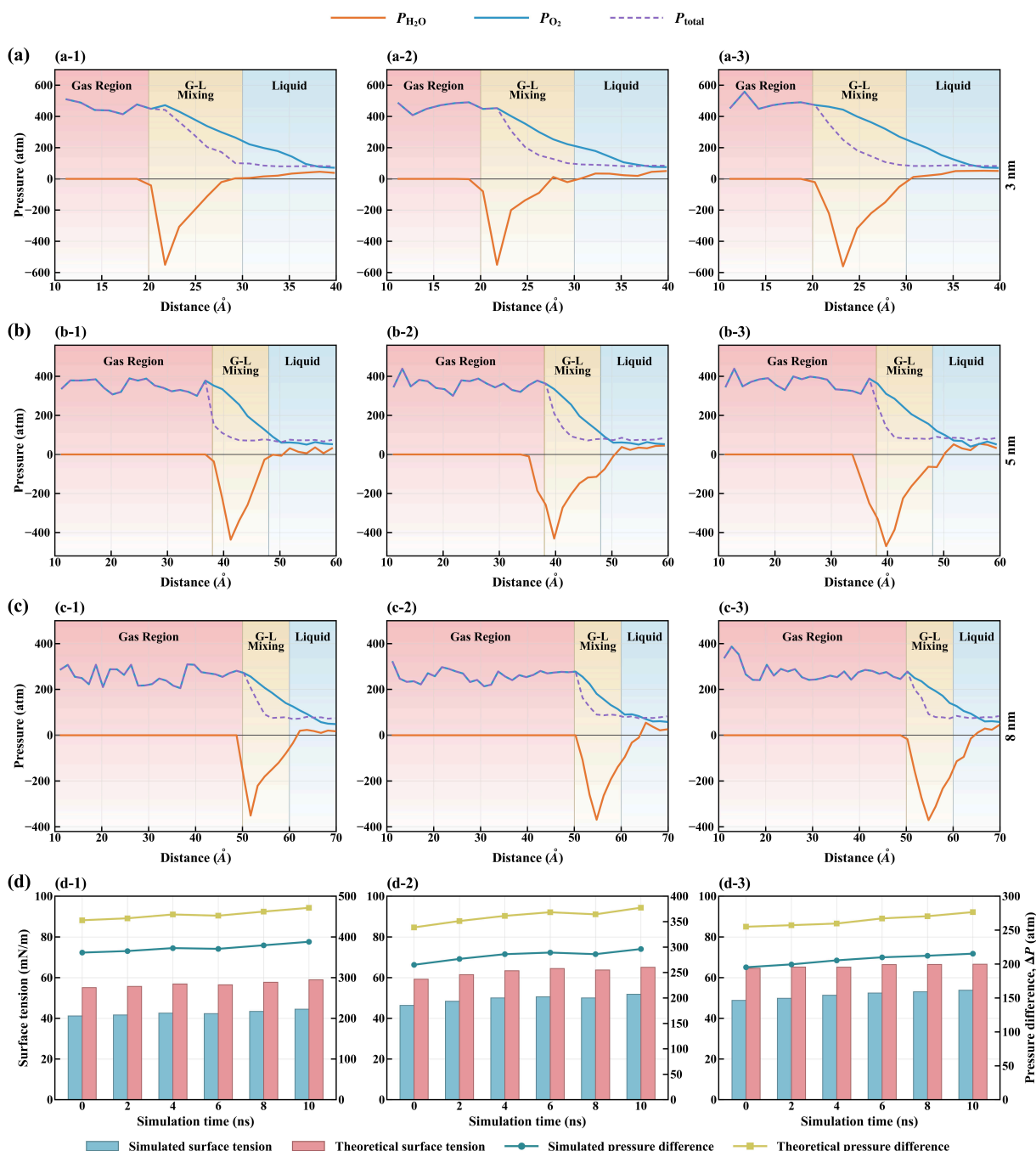


Figure 3. Size-dependent and temporal evolution of radial pressure distribution, surface tension, and pressure difference in nanobubbles. Rows (a–c) correspond to 3, 5, and 8 nm bubbles, and columns (1–3) correspond to simulation times of 0, 5, and 10 ns. Each subplot shows radial pressure profiles from the bubble center to the external water phase. The blue, orange, and purple dashed curves represent O_2 pressure, H_2O pressure and total system pressure, respectively. (d-1–d-3) compare simulated and theoretical values of surface tension and pressure difference for each bubble size. Bars (left axis) represent surface tension (blue: simulated; red: theoretical), and lines (right axis) represent internal–external pressure difference (yellow: simulated; green: theoretical). The simulated pressure difference is the actual pressure difference between the gas–liquid interface and the liquid region far from the interface, whereas the theoretical pressure difference is calculated relative to a 1 atm external reference pressure.

As shown in Figure 4c, U–T coupling energy exhibits three radial stages: plateau, peak, and fluctuation. It is close to 0 kcal/mol in the bubble core, rises rapidly in the gas–liquid transition zone to a peak range of 35–63 kcal/mol, and then decreases and continues to fluctuate in the liquid region, with a fluctuation range of approximately -37 to 30 kcal/mol. Smaller bubbles show stronger interfacial coupling energy and stronger fluctuations in the external water region. The average peak value of the 3 nm bubble is about 52 kcal/mol, 36.8% and 85.7% higher than those of the 5 and 8 nm bubbles, respectively; its fluctuation range in the liquid region is about 67 kcal/mol, 45.7% and 116.1% higher than those of the 5 and 8 nm bubbles.

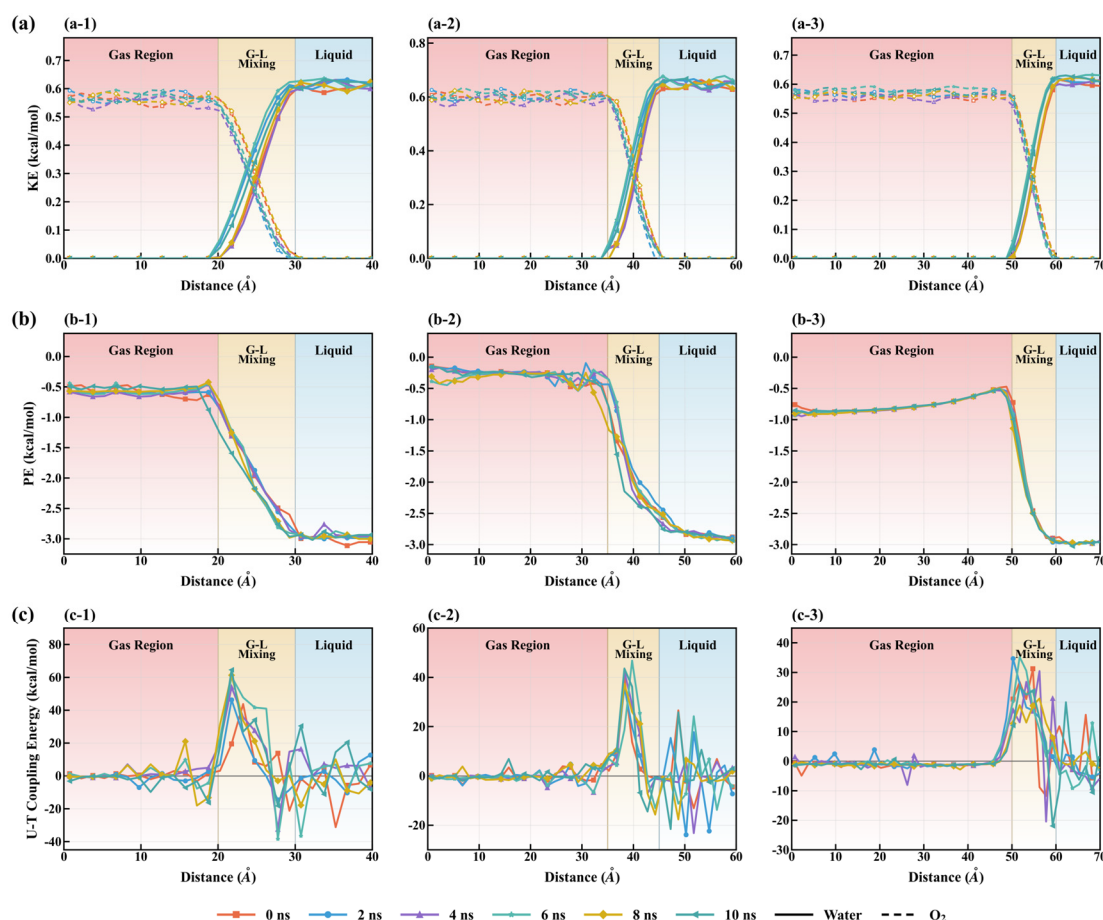


Figure 4. Size-dependent energy evolution of nanobubbles. Rows (a–c) represent kinetic energy, potential energy, and U–T coupling energy, respectively; columns (1–3) correspond to 3, 5, and 8 nm bubbles. The curves show temporal evolution of each energy term during the 0–10 ns NPT simulation.

3.4. Molecular Force Distribution Characteristics Inside and at the Interface of Bubbles

To compare local molecular dynamic characteristics among different regions, 200 molecules were randomly selected from each region to calculate velocity, net force, and force direction (Table 1). The same number of molecules was selected to maintain a consistent local sampling scale among different bubble sizes and interfacial regions and to provide basic statistical stability for force-direction percentages. This sampling was used only for molecular force and force-direction statistics; density, pressure, radius, charge, and hydrogen-bond distributions were still calculated from full-system radial spherical-shell statistics and are not limited by the 200 local molecules. For an inward-force proportion of 60–65% in the interfacial region, $n = 200$ gives an estimated 95% confidence interval of about $\pm 6.6 \pm 6.8\%$ under a binomial approximation. Therefore, this result is used to

identify a force-direction trend in the interfacial region rather than as an exact population probability. Statistical treatment and reproducibility are described in Text S3. Table 1 shows that molecular velocity increases from 345–450 m/s in the bubble core to 800–1080 m/s in the transition zone and to 744–754 m/s in the liquid region. The average net force increases from 75.25–83.23 pN in the bubble core to 371.92–421.56 pN in the gas–liquid transition zone. In terms of force direction, the bubble core and liquid region show random distributions, whereas 60–65% of the forces on oxygen and water molecules in the gas–liquid transition zone clearly point toward the bubble interior, indicating a directional constraint in this region.

Table 1. Molecular dynamic characteristics of different regions in nanobubbles with varying diameters.

Diameter	Gas Region			Gas–Liquid Mixing Region			Liquid Region		
	Velocity (m/s)	Net Force (pN)	Force Direction	Velocity (m/s)	Net Force (pN)	Force Direction	Velocity (m/s)	Net Force (pN)	Force Direction
3 nm	345	83.23	Random	800	371.92	Directed Inward (60%)	751	351.91	Random
5 nm	410	78.75	Random	915	399.75	Directed Inward (60%)	754	355.02	Random
8 nm	450	75.21	Random	1080	421.56	Directed Inward (65%)	744	353.84	Random

As bubble size increases, molecular velocity increases in different regions, whereas the average net force shows different trends. In the bubble core, the oxygen velocity of the 8 nm bubble is the highest, reaching 450 m/s, which is 30.4% and 9.8% higher than those of the 3 and 5 nm bubbles. Its average net force is the lowest, 75.21 pN, 9.6% and 4.5% lower than those of the 3 and 5 nm bubbles. In the gas–liquid transition zone, the water velocity of the 8 nm bubble is also the highest, 1080 m/s, 35.0% and 18.0% higher than those of the 3 and 5 nm bubbles. Its average net force is the largest, 421.56 pN, 13.3% and 5.5% higher than those of the 3 and 5 nm bubbles. In the liquid region, velocities (744–754 m/s) and net forces (351.91–355.02 pN) remain similar among the three bubble sizes.

Table 1 integrates the velocity, net force, and force direction statistics of molecules in different regions of nanobubbles with different diameters. The same local sample size was used for force-direction comparison, while radial distributions of density, pressure, radius, charge, and hydrogen bonds were calculated from the full system.

3.5. Charge Distribution and Hydrogen-Bond Characteristics at the Gas-Liquid Interface

Figure 5 shows the charge distribution and hydrogen-bond network characteristics both within the bubble and at the interface. In Figure 5a, the net charge along the radial distance gradually increased but decreased rapidly, exhibiting slight fluctuations within the liquid region. The net charge transitions from 0 e/Å³ in the gas region to between −0.001 and −0.0015 e/Å³ in the gas–liquid mixing region, revealing an inner-positive and outer-negative distribution. The 8 nm bubble reached a peak net charge of 0.0015 e/Å³, which was 91.1% and 65.5% higher than that of the 3 nm and 5 nm bubbles, respectively.

As shown in Figure 5b, the HBs per water molecule increased sharply with radial distance before stabilizing, expanding from 0 HBs in the gas region to 2.8–3.3 HBs in the liquid region. In the gas–liquid mixing region, the 8 nm bubble achieved an average of 3.2 HBs per water molecule, which was 17.9% and 6.5% higher than the 3 nm and 5 nm bubbles, respectively. Simultaneously, Figure 5c demonstrates that hydrogen-bond energy initially decreased rapidly before leveling off, dropping from an average of 0 kJ/mol in the gas region to between 8.2 and 9.3 kJ/mol in the liquid region. In the gas–liquid mixing region, the HB energy gradually decreased, with the 8 nm bubble reaching an HB energy of

9.3 kJ/mol, which represented a 4.49% and 13.41% higher than the 3 nm and 5 nm bubbles, respectively.

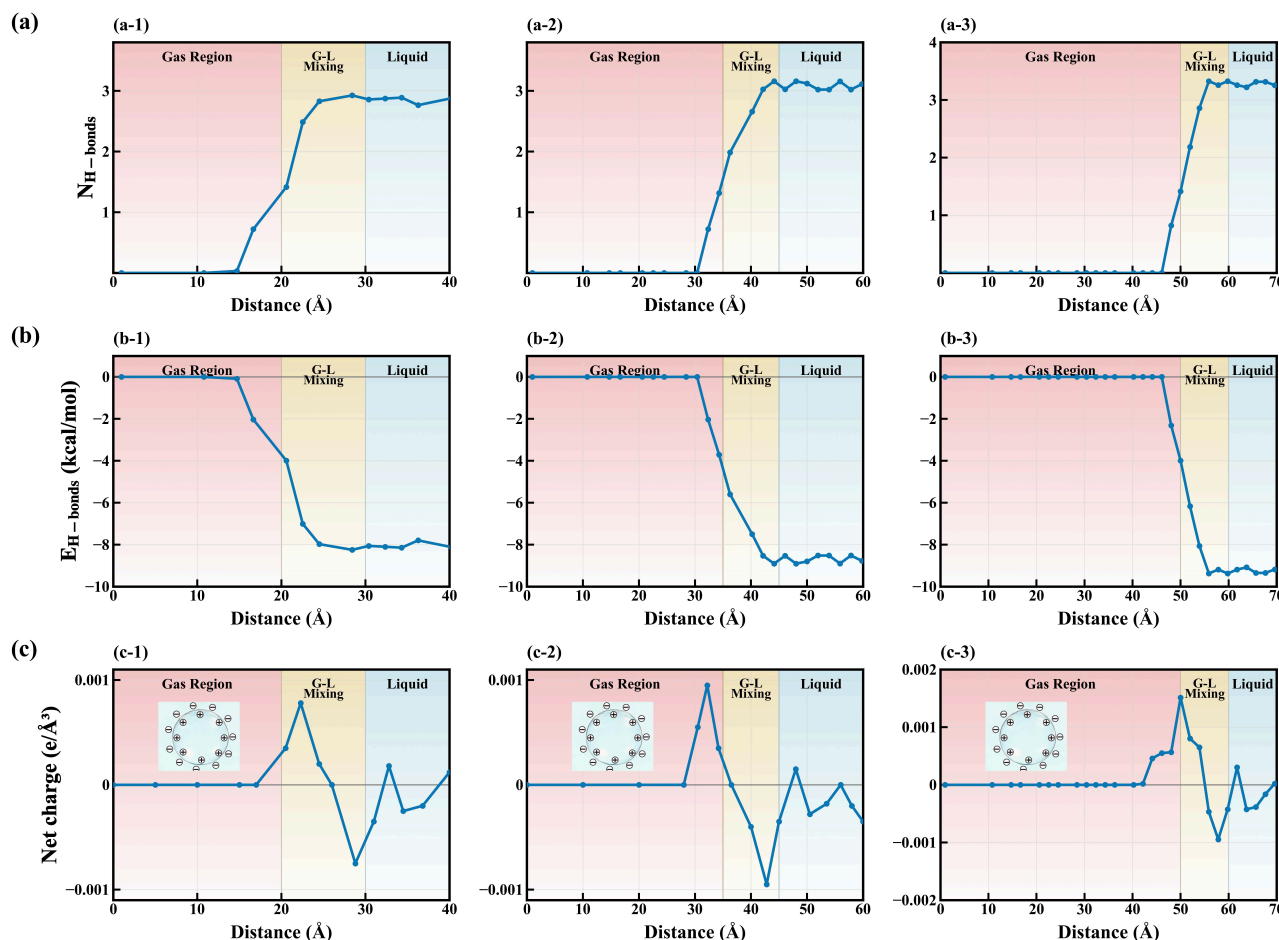


Figure 5. Radial response of interfacial hydrogen bonding and charge characteristics. Rows (a–c) represent bubble net charge, hydrogen-bond number, and hydrogen-bond energy, respectively; columns (1–3) correspond to 3, 5, and 8 nm bubbles. The curves show charge, hydrogen-bond number, and hydrogen-bond energy distributions in different radial regions at 5 ns under NPT conditions. The inset in Figure 5c schematically illustrates positive and negative charge distributions at the bubble interface.

The charge distribution and hydrogen-bond network characteristics under different water charge parameters are shown in Figure 6. Charge1–Charge4 correspond to water O/H atomic charges of $-0.60e/+0.30e$, $-0.74e/+0.37e$, $-0.84e/+0.42e$, and $-1.20e/+0.60e$, respectively. Figure 6a,b show that both net charge and hydrogen-bond number increase with the charge parameter, and Charge3 and Charge4 exhibit inner-positive and outer-negative charge distributions. The peak net charge of Charge4 reaches $0.006 e/\text{\AA}^3$, which is 37.5, 35, and 6 times those of Charge1, Charge2, and Charge3, respectively; the maximum hydrogen-bond number reaches 5.8, which is 11.6 and 1.66 times those of Charge2 and Charge3. In contrast, the water MSD in Figure 6c decreases as the charge parameter increases. Charge1 has the largest MSD, which is 11.4, 451.6, and 1303 times those of Charge2, Charge3, and Charge4. To quantify this relationship, the maximum hydrogen-bond number at 5 ns, $N_{\text{HB,max}}$, and D_{app} converted from MSD were fitted exponentially.

The core relationships are given in Equations (10) and (11), and the regression result is shown in Figure 6d:

$$D_{\text{app}} = \frac{\text{MSD}(t)}{6t}, t = 5 \text{ ns} \quad (10)$$

$$D_{\text{app}} = 1.21 \times 10^4 \exp(-1.156 N_{\text{HB,max}}) (R_{\text{ln}}^2 = 0.907) \quad (11)$$

Here, D_{app} is in $\text{\AA}^2/\text{ns}$ and $N_{\text{HB,max}}$ is the maximum hydrogen-bond number. Based on the radial hydrogen-bond distribution in Figure 6b and the MSD result in Figure 6c, the $N_{\text{HB,max}}$ values of Charge1–Charge4 are 0, 0.5000, 3.5459, and 5.8225, respectively, and the corresponding D_{app} values are 3.565×10^4 , 3.120×10^3 , 78.95, and $27.37 \text{\AA}^2/\text{ns}$. The fitting result shows that each unit increase in $N_{\text{HB,max}}$ reduces D_{app} by about 68.5%, indicating that a denser hydrogen-bond network corresponds to weaker interfacial water-molecule mobility.

Therefore, the MSD in Figure 6c characterizes the mobility of the interfacial water network rather than the long-time self-diffusion coefficient of O_2 . However, the simultaneous decrease in MSD, increase in net charge, and increase in hydrogen-bond number indicate that a dense hydrogen-bond network reduces interfacial water mobility. Because gas molecules must pass through this hydrated interfacial layer during cross-interface migration, this result provides indirect mechanistic evidence for increased interfacial transport resistance. Quantitative determination of an O_2 diffusion barrier would still require calculation of O_2 diffusion coefficients in different radial regions and hydrogen-bond lifetime distributions near the gas–liquid interface.

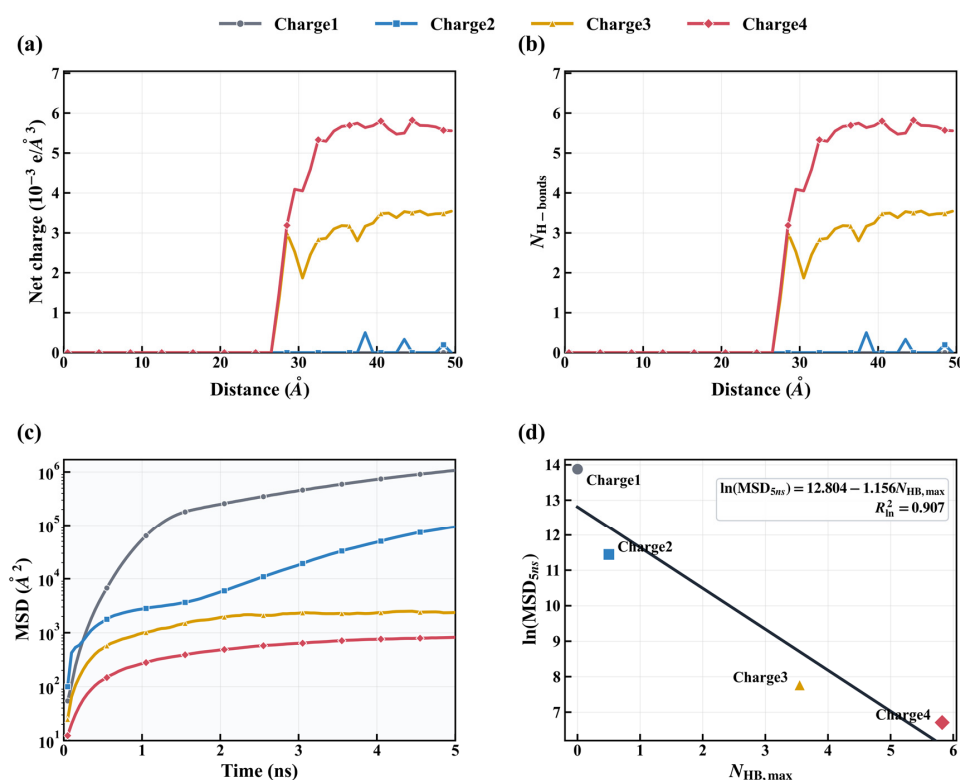


Figure 6. Interfacial properties and hydrogen-bond-MSD quantitative relationship of the 5 nm bubble under different water charge models. (a) Radial distribution of bubble net charge under different charge parameters at 5 ns; (b) radial distribution of interfacial hydrogen-bond number under different charge parameters at 5 ns; (c) time evolution of water-molecule mean-square displacement (MSD) under different charge parameters; (d) log-linear regression between maximum interfacial hydrogen-bond number and $\ln(\text{MSD}_{5\text{ns}})$. Charge1–Charge4 correspond to water O/H atomic charges of $-0.60e/+0.30e$, $-0.74e/+0.37e$, $-0.84e/+0.42e$, and $-1.20e/+0.60e$, respectively.

4. Discussion

Traditional macroscopic interfacial theory cannot explain the anomalous stability of nanobubbles, and this limitation has become a key bottleneck for micro/nano interfacial engineering. In this study, molecular dynamics simulations were used to systematically investigate the structural evolution and energy distribution of oxygen nanobubbles with diameters of 3, 5, and 8 nm in water. Classical Laplace theory regards surface tension as the core factor for bubble stability, but its applicability at the nanoscale remains questionable. Although experiments have observed the anomalous stability of nanobubbles, the underlying mechanism, including how interfacial electrostatic force, hydrogen-bond networks, and gas diffusion cooperate to regulate stability, is still unclear. Therefore, this study discusses the microscopic dominant mechanisms of nanobubble stability from three perspectives: the scale limitation of surface tension, the formation of interfacial hydrogen-bond networks, and the coupled mechanical and thermodynamic balance.

4.1. Non-Dominant Role of Surface Tension in Nanobubble Stability

Traditional bubble theory regards surface tension as the key factor that maintains bubble shape and resists expansion caused by internal pressure. At macroscopic scales, from millimeter- to micrometer-scale bubbles, this theory is usually effective: bubble rupture often occurs after rising to the gas–liquid interface, where buoyancy thins the liquid film and breaks the surface tension balance [34]. However, the present simulations reveal a distinctly different dynamic behavior at the nanoscale.

Trajectory analysis (Figure 2a) shows that nanobubbles undergo typical Brownian motion, and smaller bubbles exhibit stronger irregular motion. The 3 nm bubble has the largest motion radius during the simulation, about 3.5 nm, which is 40% and 133% larger than those of the 5 and 8 nm bubbles, respectively. This strong random diffusion dominates the bubble motion, indicating that directed buoyancy caused by density difference is negligible at the nanoscale. Thus, nanobubble destabilization does not follow the traditional rising-rupture pathway, and the stability of the interfacial structure must be analyzed in detail.

The molecular dynamics results further show that the simulated surface tension is 41–51 mN/m, systematically lower than the Laplace theoretical prediction, with deviations of 35.7% and 23.5% for the 3 and 8 nm bubbles, respectively. Therefore, this quantity is treated as an apparent surface tension derived from the local pressure difference and instantaneous radius rather than as a macroscopic equilibrium surface tension. Previous studies have also shown that nanoscale interfacial thickness, curvature correction, and molecular arrangement can cause apparent surface tension to deviate from macroscopic theoretical values [23]. Overall, surface tension still provides a basic constraint, but its individual contribution is not sufficient to explain nanobubble stability.

4.2. Formation Mechanism of Hydrogen Bond Network at the Gas–Liquid Interface in Nanobubbles

At the nanoscale, the weakening of surface tension means that other microscopic interactions must also participate. Molecular dynamics statistics show that water molecules at the gas–liquid interface experience a significant net force of 371.92–421.56 pN, with 60–65% clearly directed toward the bubble interior (Table 1). This non-random force direction reveals an asymmetric force field in the interfacial region, corresponding to the interfacial charge distribution. As shown in Figure 5a, the net charge in the gas–liquid transition zone shows an inner-positive and outer-negative distribution, with a peak value of $0.0015 \text{ e}/\text{\AA}^3$; charge and electrostatic force increase with bubble size. This conclusion is consistent with Millare and Basilia (2018) [35], who measured the interfacial potential distribution of nanobubbles in an ethanol-water system and confirmed net-charge distribu-

tion at the gas–liquid interface. MD simulations further indicate that the electrostatic effect generated by this interfacial charge structure can change the arrangement and interactions of interfacial water molecules and thereby reduce the surface tension coefficient at the gas–liquid interface [36].

Further analysis shows that hydrogen-bond formation is regulated by interfacial electrostatic strength. As the charge parameter increases, the peak net charge of Charge4 reaches $0.006\text{ e}/\text{\AA}^3$, which is 37.5, 35, and 6 times those of Charge1, Charge2, and Charge3, respectively. The maximum hydrogen-bond number reaches 5.8, which is 11.6 and 1.66 times those of Charge2 and Charge3, whereas Charge1 forms almost no hydrogen bonds. At the same time, the MSD of Charge1 is 11.4, 451.6, and 1303 times those of Charge2, Charge3, and Charge4, respectively, indicating that enhanced interfacial net charge, increased hydrogen-bond number, and restricted water mobility occur simultaneously. This result shows that interfacial electrostatic force promotes oriented water arrangement and hydrogen-bond-network densification, consistent with bulk nanobubble cluster studies showing that the electrical double layer and interfacial charge affect aggregate stability [37].

4.3. Stabilization Mechanism of Nanobubbles: Mechanical Equilibrium and Thermodynamic Dynamic Equilibrium

Nanobubble stability is first reflected in its ability to maintain morphology under high internal pressure. The simulated apparent surface tension is 42–51 mN/m, indicating that interfacial tension still provides a basic constraint, but its value is lower than the Young–Laplace prediction and is insufficient alone to explain stability. Meanwhile, radial pressure distributions (Figure 3a–c) show that pressure in the bubble core reaches 250–470 atm, whereas the external liquid region is about 90 atm, forming a pressure gradient that drives gas diffusion outward. Radial density distributions (Figure 2c–d) also show that oxygen density rapidly decreases from 0.31–0.82 g/cm³ in the core region to nearly zero along the radial direction. Under this outward-diffusion driving force, water molecules at the gas–liquid interface still experience a net force of 371.92–421.56 pN, with 60–65% directed toward the bubble interior, indicating that interfacial charge and water orientation provide additional molecular-scale constraints. Figure 4b,c further show that potential energy decreases at the interface, and U–T coupling energy reaches 35–63 kcal/mol in the gas–liquid transition zone, suggesting that this region has a stronger molecular structural response and acts as the main interfacial retardation zone during gas diffusion.

This interfacial retardation is closely related to the hydrogen-bond network. The mechanism in Figure 7 shows that interfacial charge drives directional water arrangement and forms a denser hydrogen-bond network. In Figure 6c, MSD decreases as the charge parameter increases, and the exponential relationship between $N_{\text{HB,max}}$ and D_{app} (Figure 6d) shows that when $N_{\text{HB,max}}$ increases from 0 to 5.8225, D_{app} decreases from $3.565 \times 10^4\text{ \AA}^2/\text{ns}$ to $27.37\text{ \AA}^2/\text{ns}$. This result indicates that hydrogen-bond-network densification markedly restricts interfacial water mobility and provides indirect evidence for hindered gas migration across the interface. The particle-size comparison also supports this view: the average hydrogen-bond number of the 8 nm bubble in the gas–liquid transition zone reaches 3.2 per water molecule, 17.9% and 6.5% higher than those of the 3 and 5 nm bubbles; its hydrogen-bond energy is also the highest, 9.3 kJ/mol, 4.49% and 13.41% higher than those of the 3 and 5 nm bubbles. This mechanism is consistent with recent molecular dynamics studies of nanobubble dissolution and interfacial mass transfer, in which gas migration across the interface is jointly affected by internal pressure difference, interfacial water structure, and local dynamic constraints [23,33].

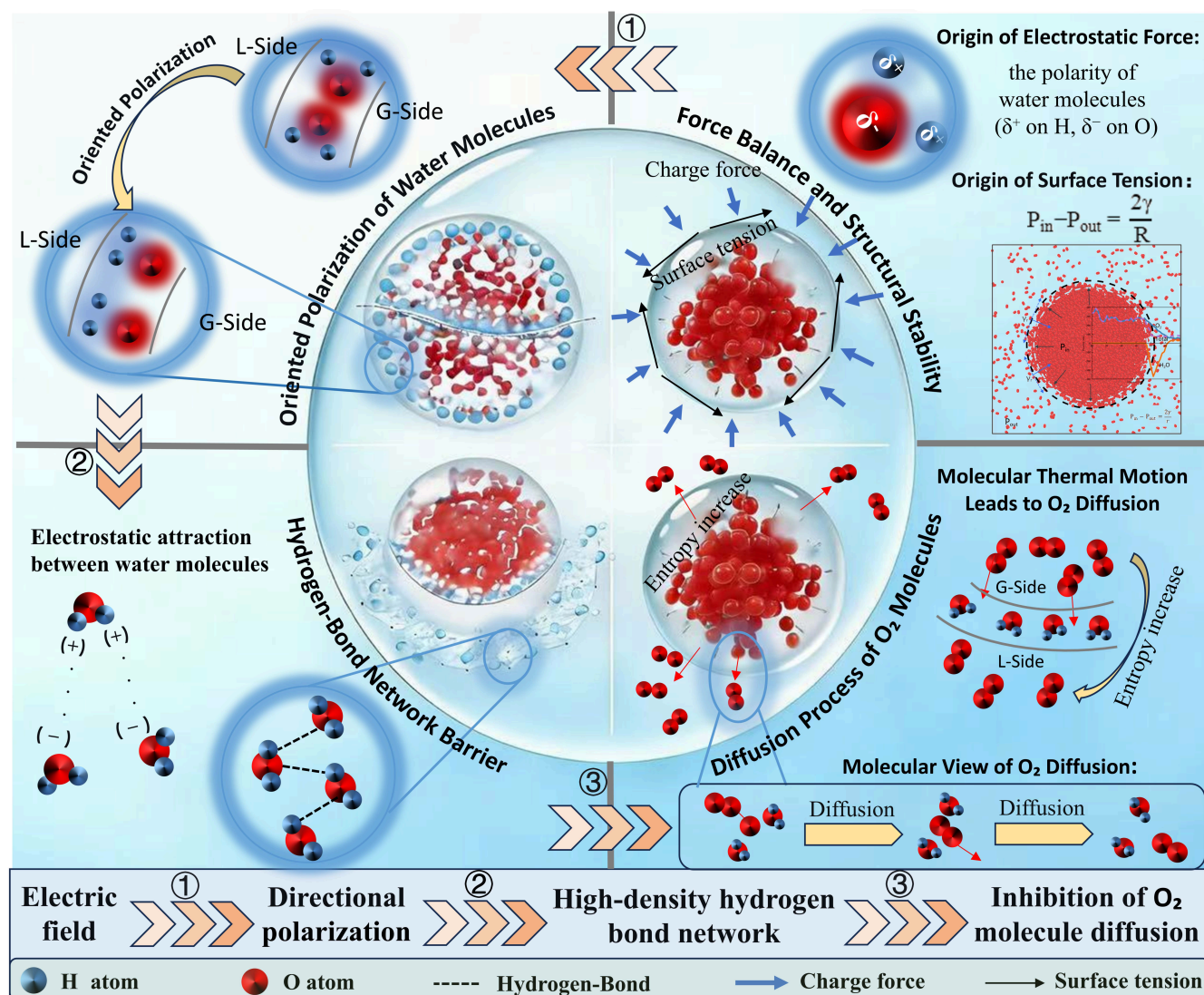


Figure 7. Mechanism diagram of nanobubble stability.

These results indicate that larger bubbles have thicker and more ordered interfacial structures, corresponding to more continuous and denser hydrogen-bond networks that significantly strengthen the retardation of gas diffusion. In contrast, smaller bubbles have larger curvature and higher internal pressure, making it difficult to form hydrogen-bond networks of comparable quality at the interface, and their structural stability is correspondingly lower. Therefore, when a bubble shrinks to a critical size, the self-regulation mechanism may fail and stability may drop rapidly. To explore this possible destabilization pathway, an auxiliary simulation was performed for a 1 nm bubble. As shown in Figure S7, this bubble exhibits typical collapse behavior: its trajectory shows abrupt contraction and sudden change at a specific time, between 7 and 8 ns, and its structure collapses within a very short time. This 1 nm simulation is used mainly to suggest a possible destabilization pathway at a critical small size and is not treated as a universal quantitative criterion for the critical size of all nanobubbles.

4.4. Limitations and Future Outlook

The present results still require further improvement in several aspects. The simulation time scale is at the nanosecond level, which is suitable for revealing early structural relaxation, interfacial molecular rearrangement, and relative evolution trends among different bubble sizes, but it cannot be directly extrapolated to hour- or day-scale long-term stability

in experiments. The current size comparison is mainly based on available production trajectories, and percentage differences should be understood as descriptive trends. Future work should perform multiple independent trajectories with different initial velocity seeds for each bubble size and extend the simulation time to obtain means, standard deviations, confidence intervals, and more reliable long-term stability assessment.

In addition, the SPC/E water model and O₂ interaction parameters can affect the absolute values of interfacial tension, diffusion behavior, and gas solubility. Other water models, such as TIP3P- or TIP4P-type models, may also change the absolute values of interfacial water structure and transport properties. Therefore, this study emphasizes relative comparisons among different bubble sizes. Regarding the mechanism by which the hydrogen-bond network hinders gas transport, the current evidence mainly comes from charge distribution, hydrogen-bond number, hydrogen-bond energy, water MSD, and morphology snapshots. These results support the mechanism of enhanced interfacial water-network constraint and restricted water mobility. Further quantitative verification of an O₂ diffusion barrier still requires calculation of O₂ diffusion coefficients in different radial regions and hydrogen-bond lifetime distributions near the gas–liquid interface.

5. Conclusions

This study used molecular dynamics simulations to systematically investigate the evolution of oxygen nanobubbles with different diameters (3, 5, and 8 nm) in water. At the molecular scale, the results reveal the size effect of nanobubbles, the cooperative stabilization mechanism of interfacial electrostatic force and apparent surface tension, and the restriction of interfacial water mobility by hydrogen-bond-network densification. The main conclusions are as follows:

(1) Bubble structural evolution shows a clear size effect. The 3 nm bubble exhibits the most pronounced curvature fluctuation, ranging from -59 to 49 nm^{-1} , with fluctuation amplitudes 3.6 and 7.2 times those of the 5 and 8 nm bubbles, respectively. Its centroid displacement is 3.5 nm, 40% and 133% larger than those of the 5 and 8 nm bubbles, indicating significantly lower structural stability for smaller bubbles.

(2) At the nanoscale, surface tension still provides a basic constraint, but its value is systematically lower than the classical theoretical prediction, with a 35.7% deviation for the 3 nm bubble, indicating that it is no longer the only dominant force maintaining bubble stability. Water molecules at the gas–liquid interface experience a net force of 371.92–421.56 pN, with 60–65% directed toward the bubble interior, forming an asymmetric force field. This force field cooperates with surface tension to maintain bubble structural stability.

(3) The asymmetric force field drives directional polarization and ordered arrangement of water molecules, inducing the formation of a high-density hydrogen-bond network. Larger water charge parameters produce stronger interfacial electrostatic force and denser hydrogen-bond networks: the peak net charge of Charge4 ($0.006\text{ e}/\text{\AA}^3$) is 37.5, 35, and 6 times those of Charge1, Charge2, and Charge3, respectively, and its hydrogen-bond number (5.8) is 11.6 and 1.66 times those of Charge2 and Charge3. This indicates that enhanced interfacial electrostatic force directly promotes hydrogen-bond-network densification.

(4) A dense hydrogen-bond network imposes clear constraints on interfacial water mobility. When the interfacial potential energy decreases, U–T coupling energy shows a 36–66 kcal/mol peak in the gas–liquid transition zone, and MSD decreases as hydrogen bonding increases. D_{app} and $N_{\text{HB,max}}$ satisfy a nearly exponential decreasing relationship (Equation (10), $R^2\ln = 0.907$), indicating that a denser hydrogen-bond network corresponds to weaker interfacial water migration ability and may increase gas-transfer resistance across the interface.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/pr14142272/s1>.

Author Contributions: M.W.: Investigation, Methodology, Software, Formal analysis, Writing—original draft. T.W.: Conceptualization, Supervision, Writing—review & editing, Funding acquisition. Y.Z.: Validation, Data curation. J.H.: Software, Visualization. M.F.: Writing—review and editing. All authors have read and agreed to the published version of the manuscript.

Funding: Supported by Jing-Jin-Ji Regional Integrated Environmental Improvement—National Science and Technology Major Project: 2025ZD1204600.

Data Availability Statement: Data are contained within the article or Supplementary Materials.

Conflicts of Interest: Author Tianzhi Wang was employed by the RuiDe ZhiChuang Innovation Technology (Tianjin) Co., Ltd. The remaining authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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