Electronic Supplementary Material (ESI) for Nanoscale Advances.


**Supplementary Information**

# Unraveling the Effects of Gas Species and Surface Wettability on Morphology of Interfacial Nanobubbles

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**Part I Supporting Figures**

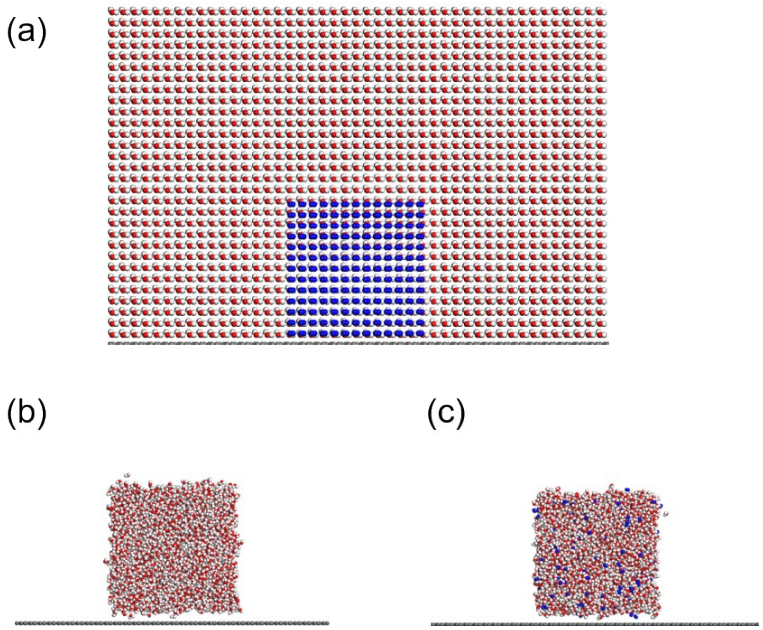


**Fig. S1** (a) Initial structure of the $H_2$ nanobubble system, which contains 57375 $H_2O$ molecules, 2197 $H_2$ molecules, and 7524 C atoms. (b) Initial state of the pure water droplet, which contains 5000 $H_2O$ molecules. (c) Initial state of the water droplet mixed with $H_2$, which contains 5000 $H_2O$ molecules and 150 $H_2$ molecules.

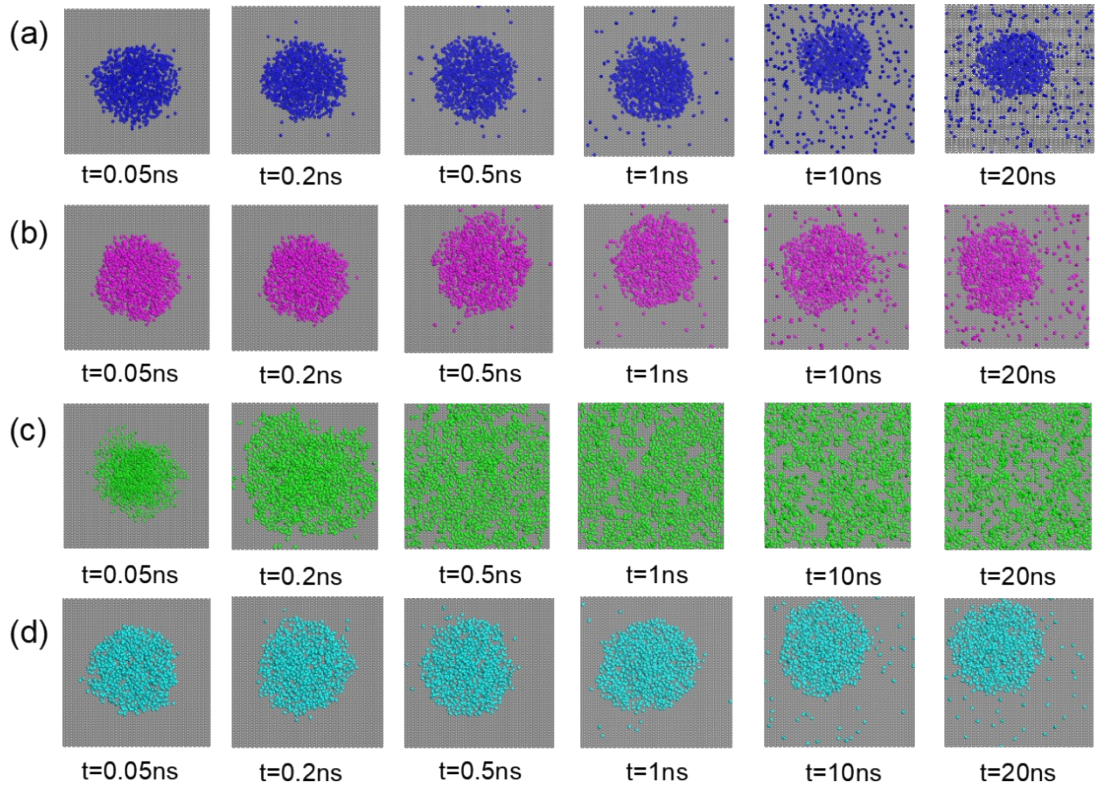


**Fig. S2** Time evolution of the (a) $H_2$, (b) $O_2$, (c) $CO_2$, and (d) $N_2$ nanocluster morphologies on atomistic flat surfaces (plan views).

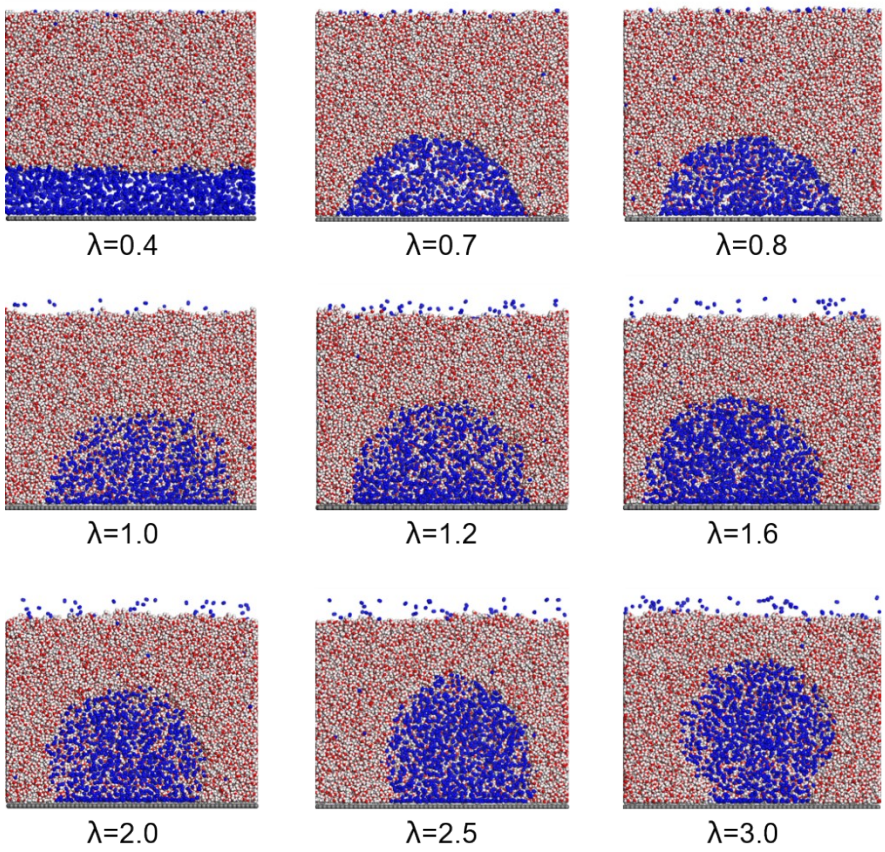


**Fig. S3** Snapshots of the nanobubbles on surfaces (side views) with different values of λ, which from small to large denotes the wettability changing from hydrophobic to hydrophilic.

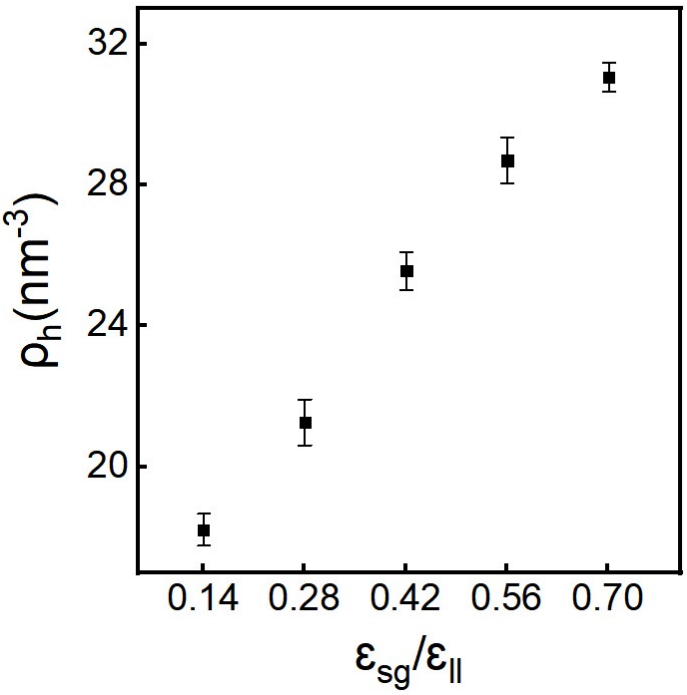


**Fig. S4** Relationship between the density of first $H_2$ layer and the interaction parameter $\varepsilon_{sg}/\varepsilon_{ll}$. Each $\varepsilon_{sg}/\varepsilon_{ll}$ is corresponding to the surfaces of different wettability from $\lambda$=0.5 to $\lambda$=2.5.

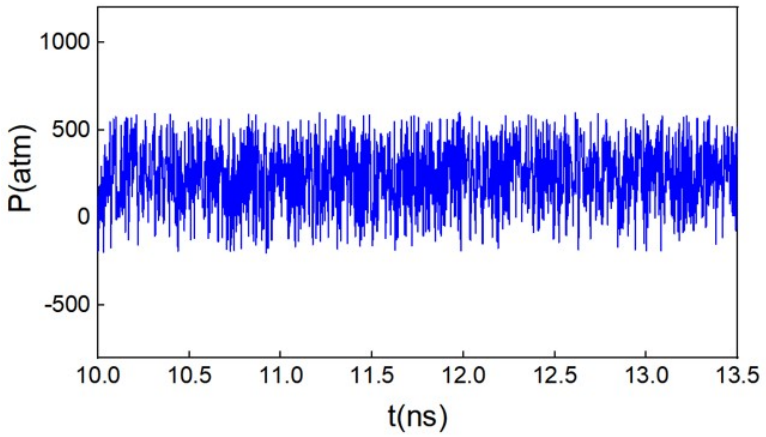


**Fig. S5** Time evolution of the internal pressure of surface nanobubble when $R_{cur}$ = 5.21 nm (λ=1.0). The pressure fluctuates a lot as the simulation goes.

**Part II Supporting tables**

**Table S1 Interaction parameters between atoms.**[1] $C_G$: the atoms of graphene; $O_W$: the O atom of $H_2O$; $H_W$: the H atoms of $H_2O$; $H_H$: the atoms of $H_2$; $O_O$: the atoms of $O_2$; $O_C$: O atom of $CO_2$; $C_C$: C atom of $CO_2$. N: N atom of $N_2$.

| | $C_G$ | $O_W$ | $H_W$ | $H_H$ | $O_O$ | $O_C$ | $C_C$ | N |
|---|---|---|---|---|---|---|---|---|
| $\mathcal{E}$(kcal/mol) | 0.086 | 0.155 | 0 | 0.022 | 0.103 | 0.103 | 0.183 | 0.074 |
| $\sigma$ (Å) | 3.400 | 3.169 | 0 | 2.683 | 3.006 | 3.006 | 2.937 | 3.292 |
| *Charge*(e) | 0 | -0.8476 | 0.4238 | 0 | 0 | -0.3256 | 0.6512 | 0 |

The water molecules are treated by the SPC/E model. The Lennard-Jones potential ($E = 4\varepsilon[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}]$) with a cutoff of 12.0 Å is employed for the Van der Waals interaction. The interaction parameters between different types of atoms are calculated through the Lorentz-Berthelot combining rules ($\varepsilon_{ij} = \sqrt{\varepsilon_{ii}\varepsilon_{jj}}$, $\sigma_{ij} = \frac{\sigma_{ii+} + \sigma_{jj}}{2}$).

## References

1 J. P. Bouanich, Site-site Lennard-Jones Potential Parameters for $N_2$, $O_2$, $H_2$, CO and $CO_2$, *J.*

*Quant. Spectrosc. RA.*, 1992, **47**,243-250.