

## **Why is the adhesion strength of hydrate only one-fifth of ice? [1]**

Rui Ma<sup>†</sup>, Feng Wang<sup>‡</sup>, Yuanhao Chang<sup>†</sup>, Senbo Xiao<sup>†</sup>, Niall English<sup>‡</sup>, Jianying He<sup>†</sup>,  
Zhiliang Zhang<sup>†</sup>

<sup>†</sup>*NTNU Nanomechanical Lab, Department of Structural Engineering, Norwegian  
University of Science and Technology (NTNU), Trondheim 7491, Norway*

<sup>‡</sup>*School of Chemical and Bioprocess Engineering, University College Dublin, Dublin  
4, Ireland*

### **ABSTRACT**

Adhesion of hydrates in pipelines often leads to catastrophic blockages, causing serious safety problems. Despite the seemingly macroscopic similarity, the adhesion strength of gas hydrate to solid surfaces is roughly only one-fifth of that of ice. Unraveling the significant difference between hydrate and ice adhesion requires a thorough understanding of the atomic adhesion of hydrates on solid surfaces and further comparisons with ice adhesion. In this work, large-scale molecular dynamics simulations (MD) are used to study the adhesion of hydrate particles on solid surfaces, with a special focus on the atomistic structures and the corresponding influences of an interfacial adhesion layer. Surprisingly, the results validate the experimental observation at the nanoscale, namely reproducing the proportional relationship between hydrate and ice adhesion strength. Specifically, the study elucidates the mechanisms underlying the adhesion difference between hydrate and ice, showing the competitive structure formation in the critical intermediate layer between hydrate and its adhering substrates. Tensile tests further directly correlate hydrate adhesion strength with different intermediate layer structures. It is found that both the lattice areal density of water structure and the adsorption of guest molecules on the solid substrate together determine the hydrate adhesion strength. These findings provide new molecular insights into hydrate adhesion and the fundamentals for the design of novel anti-hydrate surfaces.

### **REFERENCES**

[1] Ma, Rui; Wang, Feng; Chang, Yuanhao; Xiao, Senbo; English, Niall; He, Jianying; Zhang, Zhiliang. Unraveling adhesion strength between gas hydrate and solid surfaces. *Langmuir*, (2021), *accepted*.