

If Water and Methane Do Not Mix, How Do They Form Clathrate Hydrates?

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Clathrate hydrates are crystals in which water forms a network of hydrogen-bonded polyhedral cages that can be occupied by small, typically nonpolar molecules. Methane clathrates occur naturally in the permafrost and seafloor, and are the most abundant fossil fuel on Earth. Clathrates also form, unwanted, on gas pipelines, clogging them and leading to enormous economic loss. Tapping on the potential of clathrate hydrates as fuels and controlling their formation in industrial settings requires an understanding of the mechanisms by which these crystals decompose and form, as the ratio of methane to water in clathrates is 100 to 1000 times higher than the solution from which they form. This poses a puzzle: if water and methane do not mix, how do they form the clathrates? I will present work we have done in my group to elucidate the mechanism of formation of clathrate hydrates using molecular simulations.

References

(The first two papers present the models, the last 3 are on the mechanism of nucleation and growth of clathrate hydrates)

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