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Does Confinement Enable Methane Hydrate Growth at Low Pressures? Insights from Molecular Dynamics Simulations

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Natural methane hydrates are estimated to be the largest source of unexploited hydrocarbon fuel. The ideal conditions for methane hydrate formation are low temperatures and high pressures. On the other hand, recent experimental studies suggest that porous materials, thanks to their confinement effects, can enable methane hydrate formation at milder conditions, although there has not been a consensus on this. A number of studies have investigated methane hydrate growth in confinement by employing molecular simulations; however, these were carried out at either very high pressures or very low temperatures. Therefore, the effects of confinement on methane hydrate growth at milder conditions have not yet been elaborated by molecular simulations. In order to address this, we carried out a systematic study by performing molecular dynamics (MD) simulations of methane water systems. Using a direct phase coexistence approach, microsecond-scale MD simulations in the isobaric–isothermal (NPT) ensemble were performed in order to study the behavior of methane hydrates in the bulk and in confined nanospaces of hydroxylated silica pores. We validated the combination of the TIP4P/ice water and TraPPE-UA methane models in order to correctly predict the behavior of methane hydrates in accordance to their phase equilibria. We also demonstrated that the dispersion corrections applied to short-range interactions lead to artificially induced hydrate growth. We observed that in the confinement of a hydroxylated silica pore, a convex-shaped methane nanobuble forms, and methane hydrate growth primarily takes place in the center of the pore rather than the surfaces where a thin water layer exists. Most importantly, our study showed that in the nanopores methane hydrate growth can indeed take place at pressures which would be too low for the growth of methane hydrates in the bulk.

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