

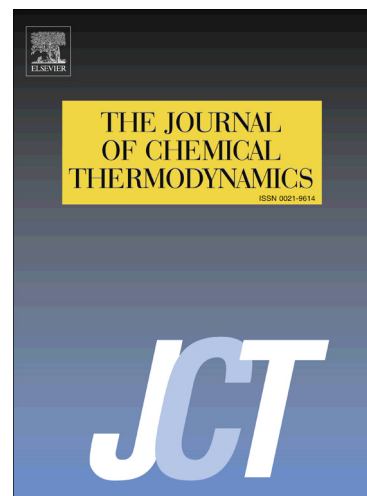
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Surface chemistry effects on heterogeneous clathrate hydrate nucleation: A molecular dynamics study

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Abstract

We report results from a molecular dynamics study of clathrate hydrate nucleation near model hydrophilic and hydrophobic surfaces. $-\text{CH}_3$ and $-\text{OH}$ terminated self-assembled monolayers (SAMs) are used as model surfaces. We study the nucleation of a soluble, structure II forming guest molecule with a coarse-grained model compatible with monatomic water. Despite the presence of SAMs, we show that nucleation occurs through a homogeneous mechanism in OHSAM and CH_3SAM systems. Formation of ice-like or intermediate water structure is not observed near either surface prior to nucleation. Nucleation occurs more quickly in OHSAM systems than CH_3SAM systems. However, the faster nucleation is driven by a partitioning of guest molecules which results in higher bulk guest concentration in OHSAM systems compared with CH_3SAM systems. Despite significant aggregation of guest molecules near CH_3SAM , no nucleation is observed near the surface. The formation of guest contact pairs, facilitated by the presence of CH_3SAM , may prevent nucleation in this region. Our results highlight the numerous routes by which surfaces can affect hydrate nucleation due to the multicomponent nature of the phenomena.

Keywords: Heterogeneous, nucleation, clathrate hydrates, molecular dynamics, simulations

1. Introduction

Clathrate hydrates are a solid phase composed of two components: water molecules that build a space-filling network of polyhedral cages through hydrogen bonding, and guest molecules that occupy some or all of these cages [1, 2, 3].
5 Clathrate hydrates are generally formed at elevated pressures (> 0.6 MPa) and low temperatures (< 300 K). Common guest molecules include light gases such as methane, ethane, and carbon dioxide, although some heavier molecules, such

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