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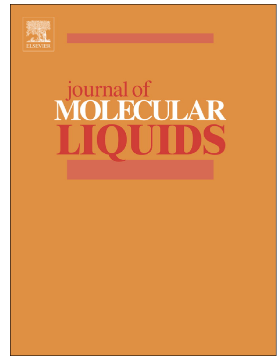

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Effect of Surface Roughness on Adsorption and Distribution of Methane at the Water-Methane Interface

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Abstract

A molecular level understanding of the structure of water-methane interface is important due to its role in methane hydrate nucleation and atmospheric chemistry. Using classical molecular dynamics simulations, we investigated the structure of water-methane interface and the adsorption of methane molecules on the water surface. The molecular level roughness of the surface and its effect on adsorption of methane are examined. An increase in the pressure is found to increase the amplitude of humps and wells on the rough water surface. The layer of methane molecules that are in direct contact with the surface and the adsorbed methane molecules above the first layer are identified. It is revealed that a greater fraction of methane molecules that are in direct contact with the surface are present at the humps than at the wells. In contrast, the density of adsorbed methane molecules above the first molecular layer of methane is found to be more above the wells. The non uniform distribution of methane adsorbed on the water surface is explained in terms of the interaction between methane and water. The distribution of adsorbed methane molecules above the water surface indicates a clear preference for the gas molecule to enter the liquid phase through the humps of the surface. The results suggest that the roughness of water surface has a crucial role in the process of methane dissolution.

1 Introduction

The structure and dynamics of the water-methane interface is an intensely researched topic due to its importance in the formation of methane hydrates. Methane hydrates are crystalline compounds in which methane molecules are encapsulated inside cavities formed by hydrogen bonded water molecules [1-3]. Methane is extracted by inducing dissociation of these hydrates and subsequent separation of dissolved methane from the hydrate melts [4, 5, 6]. Due to high capacity to store gas, hydrates are considered as an efficient means for methane storage and transportation [7]. Here, methane is allowed to form hydrate with water under suitable thermodynamic conditions. Experimentally, it was shown that the formation of hydrates occurs at the water-gas interface [8, 9]. This has been confirmed by several molecular dynamics simulation studies on hydrate nucleation