Molecular simulations of gas hydrates

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Gas hydrates are solid materials, which consist of water molecules forming cages, so that single gas molecules can be trapped into those cages. The favorable interactions between water and the guest molecules make these formations stable. Methane and Carbon dioxide are typical gases, which can form the hydrates. One of the main goals of our study is to understand the ways to extract methane as an energy source from oceanic sediments and store the carbon dioxide from the atmosphere. We study the stability of hydrates under different external conditions and with different gas inclusions with the help of Monte-Carlo adsorption simulations.