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Tunable mesoporous silica materials for gas storage applications via nanoconfined clathrate formation

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The safe storage and utilisation of gases, such as hydrogen, is an ongoing research area and has the potential to promote hydrogen as a major substitute for carbon-based fuels. Clathrates (gas hydrates) are water-based crystal structures (ice-like) able to trap hydrogen or methane molecules in the cages formed by the scaffold arrangements. As only water is required for the construction of the cages, the clathrates have been identified as a potential solution for safe gas storage. However, as the pure gas clathrate still requires harsh synthesis conditions, we propose an approach which exploits the extraordinary change of the water properties when confined in a nano-space. Specifically, it will be shown that a hydrophobic mesoporous silica can act as the nano-confinement for the ice-like hydrate. The research presented focuses on the possible surface chemistry effect of mesoporous silicas, as well as the pore network influencing the clathrate formation, showcasing applications of CH₄ and H₂ gas storage.

For example, a hydrophobized SBA-15 is demonstrated to promote methane hydrate formation [1]. In comparison to as-synthesized SBA-15, hydrophobization by C₈-grafting accelerates the kinetics of methane storage in and delivery from the hydrate. X-ray diffraction demonstrates formation of Structure I hydrate on SBA-15 C₈. At 7.0 MPa and 248 K, the water-to-hydrate conversion on hydrophobized SBA-15 C₈ reaches 96% as compared to only 71% on a pristine SBA-15 sample with comparable pore size, pore volume and surface area. Fast loading and unloading of methane on the modified silica was achieved in 19 subsequent cycles without losses in kinetics.

A Mesoporous Cellular Foam (MCF) grafted with a THF like functional group was tested for H₂ hydrate formation at 7 MPa, 262-268 K under 100% pore volume saturation of 5.56 mol% THF solution [2]. The materials exhibit rapid hydrate formation, and the THF-like functionalized MCF material showed an excellent promoting effect on H₂ storage compared to non-functionalized material MCF despite having a pore-volume \approx 16% and 24% lower than MCF, respectively.

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