# Abnormal guest exchange behavior in the sII hydrate – flue gas replacement as revealed by experimental and computational approaches for hydrocarbon recovery and $CO_2$ sequestration

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Natural gas hydrates (NGHs) have been discovered in nature, and many researchers have studied the natural gas production from NGHs because of their abundance. Particularly, the replacement process has been proposed as a promising technology that utilizes spontaneous guest exchange between $CH_4$ and $CO_2$ without the dissociation of NGHs. In this study, the abnormal guest exchange behavior in the sII ($CH_4$ + $C_3H_8$) hydrate – flue gas replacement was investigated to elucidate the cage preference of guest molecules and its impact on the lattice structure. The results showed that $N_2$ was preferentially encapsulated compared to $CO_2$ at the lower feed gas pressure, whereas the opposite tendency was observed with increasing the feed gas pressure. In addition, the MD simulation demonstrated that the characteristics of encapsulated guest molecules could differently impact the lattice of the replaced hydrates. These findings would be helpful for understanding the kinetics and mechanism of the replacement in sII hydrate using flue gas injection.