Modeling the Phase Behavior of Gas Hydrate forming Systems

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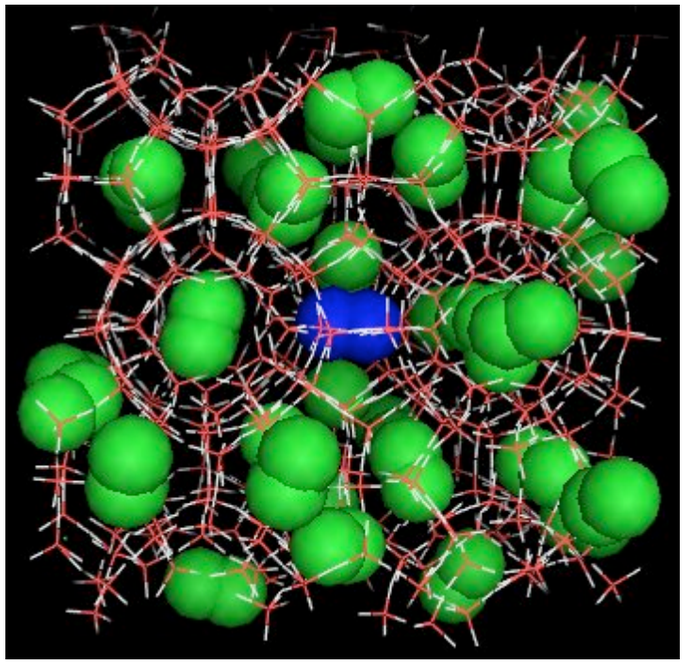
Creating a new perspective in this field, through calculations of the entire phase diagram for models of hydrate forming systems – including all fluid, ice and hydrate phases

Approach:

- Understanding role of molecular interactions in determining phase diagram

  what's the simplest molecular model that can describe hydrate stability ?

- Development of techniques for calculating free energies of hydrates using Monte Carlo simulations



Visualization of state from a Monte Carlo simulation of a structure-I ethane hydrate:

Ethane molecules in large cavities shown in green, ethane molecules in small cavities shown in blue. Probability of small cavity occupancy much lower for ethane than for methane

Role of shape of guest molecule shape in determining hydrate stability:

- study of methane, ethane and propane hydrates
- occupancies of small and large cavities in the hydrate and stability of structure-I vs. structure-II