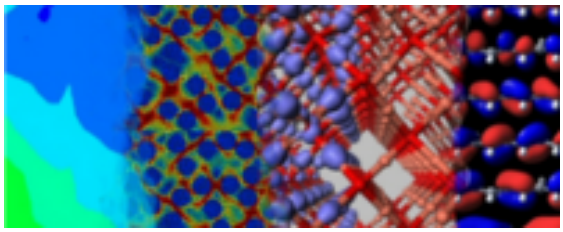

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Calculations of the free energy of sII clathrate hydrates

Friday, November 9, 2012 11:25 AM (25 minutes)

Clathrate hydrates are of great technological interest because of their capacity to store gas at relatively high density. They are therefore considered as prospective candidates for hydrogen storage materials. Extreme pressures are required to form stable pure hydrogen clathrate hydrates, which makes it impractical to use pure hydrogen clathrates in technological applications. However, the synthesis pressure of hydrogen hydrates can be significantly decreased by accommodating a second guest molecule, referred to as promoter, in the large cavities. Here we study the relationship between potential promoter molecules and the stability of binary sII hydrogen hydrates at a wide range of temperatures (233 K –293 K) by means of Monte Carlo simulations. Our aim is to predict what would be an efficient promoter molecule using properties such as size, dipole moment, and hydrogen bonding capability. The gas clathrate configurational and free energies are compared and entropy was found to make a considerable contribution to the free energy. Therefore, full free energy calculations are required to assess the stability of clathrate hydrates filled with different promoter molecules. Unfortunately, no predictive property could be distinguished.

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