

Abstract Submitted
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Hydrogen clathrate hydrates as a potential hydrogen storage material¹ DUBRAVKO SABO, JACALYN CLAWSON, SUSAN REMPE, JEFFERY GREATHOUSE, MARCUS MARTIN, KEVIN LEUNG, SAMEER VARMA, RANDALL CYGAN, TODD ALAM, Sandia National Laboratories — Recent synthetic activities involving hydrogen clathrate hydrates raised the prospect of utilizing them as an alternative storage material for hydrogen fuel. The current work is a starting point for future studies of hydrogen occupancy of hydrogen clathrate hydrate and its stability. We present studies of the structural and thermal properties of a hydrogen molecule dissolved in liquid water and their possible implication for the hydrogen storage in clathrate hydrates. The radial distribution function, coordination number and coordination number distribution are calculated using different representations of the interatomic forces within molecular dynamics, Monte Carlo and ab initio molecular dynamics simulation frameworks. Although structural details differ in the radial distribution functions generated from the different force fields, all approaches agree that the average and most probable number of water molecules occupying the inner hydration sphere around hydrogen is 16. Furthermore, we estimate the hydrogen hydration free energy. In addition, we will present the quantum mechanical studies of the hydrogen occupancy in single clathrate hydrate cages.

¹DOE

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