

Abstract Submitted
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First-principles stability study of clathrate hydrates under pressure TIMO THONHAUSER, QI LI, BRIAN KOLB, Wake Forest University — We present a first-principles DFT study of the structural stability of clathrate hydrates under pressure. These materials form under high pressure and low temperature and consist of polyhedral water cages that form an ice-like framework of hydrogen bonds. Clathrate hydrates can be filled with guest molecules such as methane or molecular hydrogen, in which case these materials and their stability are of interest for energy-storage solutions. Since the interactions between the water molecules themselves—but also between the water molecules and the guest molecules—is at least partly determined by van der Waals forces, we utilize the recently developed self-consistent van der Waals density functional vdW-DF (T. Thonhauser, V.R. Cooper, S. Li, A. Puzder, P. Hyldgaard, and D.C. Langreth, Phys. Rev. B 76, 125112 (2007)). For our simulations we consider the empty host lattice, as well as the host lattice filled with methane and molecular hydrogen, for pressures up to 1 GPa. Our results show that the system undergoes phase transitions from *structure I* to *structure II* and finally to *structure H*, in good agreement with experiment.

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