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Predicted novel hydrogen hydrate structures under pressure from first principles GUANGRUI QIAN, ANDRIY LYAKHOV, QIANG ZHU, ARTEM OGANOV, XIAO DONG, State Univ of NY- Stony Brook — Gas hydrates are systems of prime importance. In particular, hydrogen hydrates are potential materials of icy satellites and comets, and may be used for hydrogen storage. We explore the H2O-H2 system at pressures in the range $0 \sim 100$ GPa with ab initio variable-composition evolutionary simulations. According to our calculation and previous experiments, the H2O-H2 system undergoes a series of transformations with pressure, and adopts the known open-network clathrate structures (sII, C0), dense "filled ice" structures (C1, C2) and two novel hydrogen hydrate phases. One of these structures is based on the hexagonal ice framework and has the same H2O:H2 ratio (2:1) as the C0 phase at low pressures and similar enthalpy (we name this phase Ih-C0). The other newly predicted hydrate phase has a 1:2 H2O:H2 ratio and structure based on cubic ice. This phase (which we name C3) is predicted to be thermodynamically stable above 38 GPa when including van der Waals interactions and zero-point vibrational energy. This is the hydrogen-richest hydrate and this phase has the highest gravimetric densities (18 wt.%) of extractable hydrogen among all known materials. We thank the DARPA (Grants No. W31P4Q1310005 and No. W31P4Q1210008), National Science Founda- tion (EAR-1114313, DMR-1231586), AFOSR (FA9550-13-C-0037), DOE (DE-AC02-98CH10886), CRDF Global (UKE2-7034-KV-11) for financial support. We thank Purdue University Teragrid for providing computational resources and technical support for this work (Charge No.: TG-DMR110058).

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