

Abstract Submitted
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Quantum Monte Carlo simulations of high pressure solid hydrogen JONATHAN LLOYD-WILLIAMS, BARTOMEU MONSERRAT, PABLO LOPEZ RIOS, University of Cambridge, NEIL DRUMMOND, Lancaster University, RICHARD NEEDS, University of Cambridge — Several solid phases of hydrogen have been observed but the stable structures of hydrogen at high pressure remain experimentally undetermined because of the weak scattering of protons in x-ray diffraction studies. Theoretical identification of the structures is also difficult because of the small energy differences between competing phases and the large zero-point (ZP) contributions to the energies. We have performed static-nucleus diffusion Monte Carlo calculations for the candidate high pressure phases across a range of relevant densities and added ZP energies from both harmonic and anharmonic density functional theory calculations. We have used our calculated total energies to construct an enthalpy-pressure phase diagram from which we have evaluated the relative stability of the candidate structures.

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