

Abstract Submitted
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The liquid-liquid phase transition in dense hydrogen¹ DAVID CEPERLEY, Univ of Illinois - Urbana Champaign, CARLO PIERLEONI, University of L'Aquila, Italy, MARKUS HOLZMANN, CNRS, Grenoble, France, MIGUEL MORALES, Lawrence Livermore National Laboratory — The phase diagram of high pressure hydrogen is of great interest for fundamental research. A first-order phase transition in the fluid phase between a molecular insulating fluid and a monoatomic metallic fluid has been long anticipated. Recent experiments reported contrasting results about the location of the transition and theoretical results are very uncertain. We report highly accurate coupled electron-ion quantum Monte Carlo calculations of this transition, finding results that lie between the two experimental predictions, close to that measured in diamond anvil cell experiments but at 25-30 GPa higher pressure. The transition along an isotherm is signaled by a discontinuity in the specific volume, a sudden dissociation of the molecules, a jump in electrical conductivity and loss of electron localization. For details see Proc. Nat. Acad. Sc. 113, 49534957, 2016.

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