

Abstract Submitted
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First-principles study of the effect of helium on the onset of dissociation in liquid hydrogen KYLE CASPERSEN, SEBASTIEN HAMEL, TADASHI OGITSU, FRANÇOIS GYGI, University of California Davis, ERIC SCHWEGLER, Lawrence Livermore National Laboratory — The onset of molecular dissociation in liquid hydrogen under high-pressures is known to occur abruptly, possibly involving a first-order liquid-liquid phase transition [1,2]. We have examined this transition in detail by performing a series of large-scale first-principles molecular dynamics simulations of liquid hydrogen and mixtures of hydrogen with small concentrations of helium. In addition, we have examined the electronic properties of hydrogen-helium mixtures by using hybrid density functional theory to analyze snapshots from our molecular dynamics simulations. This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48. [1] S. Scandolo, PNAS 100, 3051 (2003). [2] S.A. Bonev, et al. Phys. Rev. B 69, 014101 (2004).

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