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First-principles study of the effect of helium on the onset of dissociation in liquid hydrogen KYLE CASPERSEN, Lawrence Livermore National Laboratory, FRANCOIS GYGI, University of California Davis, ERIC SCHWEGLER, Lawrence Livermore National Laboratory — The molecular to non-molecular liquid-liquid phase transition that occurs in high-temperature/high-pressure hydrogen has been speculated to be first-order-like, where the onset of dissociation occurs abruptly. However, a small concentration of non-interacting particles, specifically helium, has been postulated to retard and smooth the transition. To study this transition in hydrogen and hydrogen-helium mixtures we performed a series of large-scale Born-Oppenheimer molecular-dynamic simulations. Additionally, we have studied the electronic properties of hydrogen-helium mixtures by using hybrid density functional theory to analyze snapshots from our molecular dynamics simulations. The simulations show that the transition is smooth and continuous without any indication of any first-order-like behavior. The simulations also predict that small concentrations of helium have a significant effect on the phase transition; most notably, the pressure profile is much smoother, and the band gap closes at a higher temperature, for the hydrogen-helium mixtures relative to pure liquid-hydrogen. 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.

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