Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

High pressure bonding properties of hydrogen[1] ISAAC TAMBLYN, Dalhousie University, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, STANIMIR BONEV, Dalhousie University — There has been considerable experimental and theoretical effort to describe the transition in hydrogen from a molecular to non-molecular fluid. Resolution of discrepancies that continue to exist between different investigations of hydrogen is expected to have significant implications in fields such as planetary science. We have preformed three sets of first-principles simulations, constant density, pressure, and temperature, in order to study the molecular, non-molecular, and transition regimes of the hydrogen (deuterium) phase diagram. Constrained and unconstrained bond length simulations were used to examine changes that occur in the inter-atomic potential upon disassociation. By forcing the destruction of molecules in the molecular regime, and by considering the catalyzing effect of single hydrogen atoms, we have probed the mechanisms that drive this transition. Finally, spatial distributions of species surrounding molecules at the time of dissociation have provided insight into the structure of the liquid.

[1]Work supported by the NSERC of Canada. E.S. worked under the auspices of the U.S. Dept. of Energy at the University of California/LLNL under contract No. W-7405-Eng-48

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Date submitted: 20 Nov 2006 Electronic form version 1.4