Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Prediction of a superionic phase of hydrogen fluoride (HF) at high temperature and pressure[1] LAURENCE FRIED, NIR GOLDMAN, Lawrence Livermore National Laboratory — We report first principles simulations of hydrogen fluoride. Ab initio molecular dynamics simulations of HF were conducted at densities of 1.8 – 4.0 g/cc along the 900 K isotherm. At experimentally observable conditions, we find a transition to a superionic phase, in which the fluorine ions exhibit a stable lattice and the hydrogen ions exhibit rapid diffusion. This phase is similar to the recently reported superionic phase in water, in that there is a symmetrization of the hydrogen bond, and we observe a transient partially covalent network at pressures greater than 66 GPa. In addition, we describe a mechanism for hydrogen diffusion through the fluorine sub- lattice. Our results provide evidence that superionic solids are prevalent in solids that manifest low temperature symmetric hydrogen bonding. The pressures needed to induce superionic diffusion in HF are significantly lower than what is required for other known superionic hydrides, and thus will permit much more extensive experimental studies of this exotic phase.

[1]This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

Laurence Fried
Lawrence Livermore National Laboratory

Date submitted: 29 Nov 2005 Electronic form version 1.4