Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Dynamic structure of superionic protons in hydrogen fluoride crystal YOSHIYUKI OHDE, KAZUO TSUMURAYA, Meiji University, Kanagawa, Japan — Hydrogen fluoride crystal forms zig-zag chains of hydrogen fluoride molecules forming covalent bond between them. Goldman et al.(J. Chem. Phys.125,044501(2006).) have found the superionic state of the protons in the hydrogen fluoride crystal at 900 K and beyond the pressures at 33 GPa. The present study elucidates the dynamic structure of the protons in the superionic state of the crystal at the extreme conditions with the first principles molecular dynamics method. The strong covalent bond between the proton and the fluorine in the conductor has shown a different dynamic structure from that in the α-CuI; The protons in the conductor are bonded with the nearest fluorine and the other protons are located at incommensurate sites of the bcc fluorine lattice. This is a different dynamic structure from the formation of the incommensurate dynamic copper dimers in the α-CuI.(Tsumuraya *et al*. J. Phys. Soc. Jpn. 81,055603(2012).)

Yoshiyuki Ohde
Meiji University, Kanagawa, Japan

Date submitted: 08 Nov 2012 Electronic form version 1.4