

Abstract Submitted  
for the DPP06 Meeting of  
The American Physical Society

**Density Functional Theory simulations of water: phase-diagram and electrical conductivity** THOMAS R. MATTSSON, MICHAEL P. DESJARLAIS, Sandia National Laboratories — Knowledge of the properties of water is essential for correctly describing the physics of giant planets as well as shock waves in water. By using finite temperature density functional theory (DFT) we have investigated the structure and electronic conductivity of water across three phase transitions (molecular liquid/ ionic liquid/ superionic/ electronic liquid). There is a rapid transition to ionic conduction at 2000 K and 2 g/cm<sup>3</sup> while electronic conduction dominates at temperatures at and above 6000 K. We predict that the fluid bordering the superionic phase is conducting above 4000 K and 100 GPa [1]. Earlier work instead has the superionic phase bordering an insulating fluid, with a transition to metallic fluid not until 7000 K and 250 GPa. The LDRD office at SNL supported this work. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

[1] T.R. Mattsson and M.P. Desjarlais, Phys. Rev. Lett. 97, 017801 (2006).

Thomas R. Mattsson  
Sandia National Laboratories

Date submitted: 31 Jul 2006

Electronic form version 1.4