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Electrical conductivity of shocked water from Density Functional Theory THOMAS R. MATTSSON, MICHAEL P. DESJARLAIS, Sandia National Laboratories — We present Density Functional Theory (DFT) calculations of water in a region of phase space of interest in shock experiments. The onset of electrical conductivity in shocked water is determined by ionic conductivity, with the electron contribution dominating at higher pressures. The ionic contribution to the conduction is calculated from proton diffusion (Green-Kubo formula) and the electronic contribution is calculated using the Kubo-Greenwood formula [1]. The calculations are performed with VASP, a plane-wave pseudopotential code. At 2000K and a density of 2.3 g/cc, we find a significant dissociation of water into H, OH, and H3O, not only intermittent formation of OH - H3O pairs as suggested earlier for 2000 K and 1.95 g/cc [2]. The calculated conductivity is compared to experimental data [3]. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Safety Administration under contract DE-AC04-94AL85000. This project was supported by the Sandia LDRD office. [1] M. P. Desjarlais, J. D. Kress, and L. A. Collins; Phys. Rev. B **66**, 025401 (2002). [2] E. Schwegler, et al. Phys. Rev. Lett. **87**, 265501 (2001). [3] P.M. Celliers, et. al. Physics of Plasmas **11**, L41 (2004).

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