

Abstract Submitted  
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**Dielectric constant of water under deep Earth pressures and temperature conditions**<sup>1</sup> DING PAN, LEONARDO SPANU, Department of Chemistry, University of California, Davis, FRANCOIS GYGI, Department of Computer Science, University of California, Davis, GIULIA GALLI, Department of Chemistry, University of California, Davis; Department of Physics, University of California, Davis — The knowledge of the dielectric constant of water as a function of pressure (P) and temperature (T) plays a critical role in understanding the chemistry of aqueous systems, and in particular of fluids in the Earth mantle, where water is stored in hydrous minerals. By using first-principles molecular dynamics, we have computed the dielectric constant of water at  $T = 1000$  K, between 1 and 10 GPa, under conditions of the Earth upper mantle. We present a detailed comparison of our results with available experimental data and empirical models, and we discuss how the liquid dielectric constant is affected by the changes in the hydrogen-bond network and molecular dipole moment observed upon compression.

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