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Dielectric properties of water and their impact on the Earth's deep carbon cycle[1] DING PAN, Department of Chemistry and Department of Physics, University of California Davis, Davis, CA 95616, LEONARDO SPANU, Department of Chemistry, University of California Davis, Davis, CA 95616, BRANDON HARRISON, DIMITRI SVERJENSKY, Department of Earth & Planetary Sciences, Johns Hopkins University, Baltimore, MD 21218, GIULIA GALLI, Department of Chemistry, University of California Davis, Davis, CA 95616; Department of Physics, University of California Davis, Davis, CA 95616 — 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's mantle. By using *ab initio* molecular dynamics, we computed the dielectric constant of water at T = 1000 and 2000 K, between 1 and 12 GPa, under conditions of the Earth's upper mantle. By comparing our results with available experimental data and empirical models, we discuss how the changes in the molecular dipole moments and hydrogen-bond network upon compression affect the dielectric constant of the liquid. Based on the calculated dielectric constants, the solubility products of carbonate minerals were predicted. At P $\sim$ 10 GPa and T = 1000 K, we found that $MgCO_3$ (magnesite) is slightly soluble in water at the millimolal level, which suggests that water in the Earth's mantle has the capacity to store and transport significant quantities of oxidized carbon.

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