MAR14-2013-020078

Abstract for an Invited Paper
for the MAR14 Meeting of
the American Physical Society

Dielectric Properties of Water Under Extreme Conditions[1]

DING PAN, Department of Chemistry, University of California Davis, Davis, CA 95616

Water is a major component of fluids in the Earth's mantle, where its properties are substantially different from those at ambient conditions. At the pressures and temperatures of the mantle, experiments on aqueous fluids are challenging, and several fundamental properties of water are poorly known; e.g., its dielectric constant has not been measured. This lack of knowledge of water dielectric properties has greatly limited our ability to model water-rock interactions and, in general, our understanding of aqueous fluids below the Earth's crust. Using ab initio molecular dynamics, we computed the dielectric constant of water under the conditions of the Earth's upper mantle, and we predicted the solubility products of carbonate minerals [1]. We found that $MgCO_3$ (magnesite)—insoluble in water under ambient conditions—becomes at least slightly soluble at the bottom of the upper mantle, suggesting that water may transport significant quantities of oxidized carbon. We also computed the electronic dielectric constant of water as a function of pressure [2] and we found that, contrary to expectations based on widely used simple models, both the refractive index and the electronic band gap of water increase under pressure.

[1] D. Pan, L. Spanu, B. Harrison, D. A. Sverjensky and G. Galli, Proc. Natl. Acad. Sci. U. S. A. 110, 6646 (2013)
[2] D. Pan. Q. Wan, G. Galli (submitted for publication)

[1]The work is supported by DOE-CMCSN under Grant DE-SC0005180 and by the Sloan Foundation through the Deep Carbon Observatory.