

Abstract Submitted
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First-principles Raman spectroscopy of dissolved carbon in water under extreme conditions¹ DING PAN, Department of Physics and Department of Chemistry, Hong Kong University of Science and Technology, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago; Argonne National Laboratory — The aqueous properties of dissolved carbon at extreme conditions are of great importance to the carbon cycle in the deep Earth, which substantially influences the carbon budget near the Earth's surface, and in turn global climate change. We carried out first-principles simulations that showed that, contrary to the assumptions of many geochemical models, carbon dissolved in water-rich fluids at the bottom of the Earth's upper mantle is not in the form of CO₂(aq) but rather in carbonate and bicarbonate ions [1]. We also calculated the Raman spectra of (bi)carbonate aqueous solutions at supercritical conditions, and obtained the Raman scattering cross sections of carbon species at high pressures and high temperatures from first principles. We will discuss how to use our results to interpret and guide spectroscopic measurements. [1]D. Pan and G. Galli, *Sci. Adv.* 2, e1601278(2016)

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