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STRUCTURE, ENERGETICS, AND ELASTICITY OF HYDROUS PHASES

MOOKHERJEE, Mainak¹, PENG, Ye¹, HOSSAIN, Kariza¹ and HERMANN, Andreas², (1)Earth, Ocean and Atmospheric Sciences, Florida State University, Tallahassee, FL 32306, (2)School of Physics and Astronomy,, The University of Edinburgh, James Clerk Maxwell Building, Edinburgh,, EH9 3FD, United Kingdom, mmookherjee@fsu.edu

Among all other terrestrial planets, Earth is unique- it has surface water that is a crucial ingredient for making it a habitable planet. Water also plays an important role in sustaining geological activities. For example water helps facilitating melting by affecting the melting temperatures of silicate rocks. Water also affects rheological properties in the deep Earth and without water it would be difficult to sustain the mantle convection. Thus it is important to know how much water is there in the solid Earth and how is water transported in the deep Earth. It is well known, that water is transported in the deep Earth by suite of hydrous phases. However, to determine how much water is transported and how pervasive is the mantle hydration, it is crucial for us to map out mantle hydration by getting better constraints from seismological observations. This however relies on better constraints on resolving the differences between the elastic properties of hydrous phases from the dominant mantle phases. Elasticity of mantle phases have been extensively researched, however, our understanding of the elasticity of hydrous phases are limited and requires further investigation.

High-pressure experiments and *first-principles* simulations based on density functional theory (DFT) have been crucial in enhancing our understanding of hydrous phases that are likely to be present in the Earth's mantle and subduction zones. In this study, we present DFT results and compare them with experimental studies. In particular, we provide constraints on the crystal structure, thermodynamic stability, equation of state, elasticity of hydrous phases, and the degree of mantle hydration.

Session No. 24

[T15. Mineral Physics Research Aspects Related to Deep Earth's Interior and Phenomena I](#)

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