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Exploration of the deep Earth water cycle: a collaboration of first-principles calculations and synchrotron x-ray diffraction studies

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Water at the Earth's surface is believed to be transported into the Earth's interior by hydrous minerals. Until recently, however, hydrous minerals were not thought to persist at the extremely high-pressure conditions of the Earth's lower mantle (e.g., 23-120 GPa). In recent years, hydrous phases such as phase H (MgSiO4H2), pyrite-type FeOOH, and delta-AlOOH have been found to be thermodynamically stable at lower mantle pressures. First-principles studies have played an essential role in identifying these new phases and determining their geophysical properties (compressibility, elastic modulus, sound velocity, etc.), as well as providing the necessary parameters required to support the experimental identification of these high-pressure polymorphs using synchrotron radiation experiments. First-principles calculations suggest that the hydrous minerals stable at lower mantle pressure conditions (i.e., phase H, FeOOH, and AlOOH phases) all have symmetric hydrogen bonds. This suggests that the strength of hydrogen bonds is closely related to the stability and physical properties of hydrous minerals under pressure. This presentation summarizes recent theoretical and experimental studies of hydrous minerals that are stable at extreme pressures with a focus on the important role of hydrogen bonding [1]. This abstract is one of contributions from Commission of Physics of Minerals (CPM), International Mineralogical Association (IMA).

References

[1] J. Tsuchiya and E. C. Thompson, Progress in Earth and Planetary Science 9, 63, 10 (2023).

Primary author: TSUCHIYA, Jun (Geodynamics Research Center, Ehime University)

Co-author: Dr THOMPSON, Elizabeth C. (Department of Earth and Environmental Systems, Sewanee, The University of the South)

Presenter: TSUCHIYA, Jun (Geodynamics Research Center, Ehime University)

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