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High pressure-temperature proton migration in P-3 brucite [$Mg(OH)_2$]: Implication for electrical conductivity in deep mantle

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The recycling of water in deep earth is one of the major concerns in earth sciences. Hydrous minerals contribute largely to the transport and distribution of water into the Earth's mantle to regulate the process of deep-water cycle. Brucite is one such intriguing yet the simplest dense hydrous mineral phase belonging to MgO-SiO_2-H_2O ternary system, which contains significant amount of water in the form of OH^- groups [1], spanning a wide range of pressure stability. Simultaneously, the pressure (*p*) and temperature (*T*) induced mobility of protons within the layered structure of brucite is crucial for consequences on electrical conductivity of the mantle. Using ab initio molecular dynamics (AIMD) simulations, we investigate the diffusion of H in high-pressure trigonal P-3 polymorph of brucite [2] in a combined *p-T* range of 10-85 GPa and 1000-2000K, relevant to the Earth's mantle. The AIMD simulations reveals an unusual pressure-dependence of the proton migration in brucite characterized by maximum H-diffusion in the pressure range of 72-76 GPa along different isotherms. We predict that in the P-3 brucite phase the H mobility is onset only when a critical hydrostatic pressure is attained. The onset pressure is observed to drop with increasing temperature. The diffusion in brucite phase at elevated *p-T* takes place in such manner so that the process results in amorphization of the H-sublattice, without disturbing the Mg- and O-sublattices. This selective amorphization yields a pool of highly mobile protons causing a subsequent increment in the electrical conductivity in P-3 brucite. Our calculated values of conductivity are compared with ex-situ geophysical magnetic satellite data [3] indicating that brucite can be present in larger quantity in the lower mantle than it was previously observed. This hydroxide phase can occur as segregated patches between the dominant constituents e.g., silicates and oxides of the lower mantle and thus can explain the origin of high electrical conductivity therein.

[1] Guo X and Yoshino T 2014 *Geophys. Res. Lett.* **41** 813–9

[2] Mookherjee M and Stixrude L 2006 *Am. Mineral.* **91** 127–34

[3] Constable S and Constable C 2004 *Geochemistry, Geophys. Geosystems* **5** 1–15