

First principles investigation on hydrogen diffusivity in hydrous wadsleyite under high pressure

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Wadsleyite is thought to be a primary constituent in the upper part of the Earth's transition zone and this phase can be a significant water reservoir in the Earth. We have investigated and clarified the high pressure structural and elastic properties of hydrous wadsleyite using first principles calculation. We demonstrated that our structural models show good agreements with high pressure experimental studies and the seismic velocities of hydrous wadsleyite decrease almost linearly with increasing the degree of hydration. For the next step, we have also calculated hydrogen diffusivity of hydrous wadsleyite using our structural models. Using these results, we discuss the effects of water on the mantle dynamics.

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