

## **First-principles study of hydrogen bond symmetrization of phase D under high pressure**

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### **ABSTRACT**

We have investigated the physical and structural properties of phase D ( $\text{MgSi}_2\text{O}_6\text{H}_2$ ) at high pressure by means of a first-principles calculation method. Phase D is important as a dense hydrous magnesium silicate with high stability under pressure, and as one of the most likely candidates for a water reservoir in the Earth's lower mantle. The calculated compression behavior of phase D is in very good agreement with experimental results. We found a distinct but continuous change from asymmetric to symmetric hydrogen bonding in phase D at 40 GPa. This pressure-induced hydrogen bond symmetrization has a significant effect on the compression behavior of phase D. The bulk modulus increases by about 20% with this structural change. This behavior of pressure-induced hydrogen bond symmetrization is very similar to that previously reported by us for  $\delta\text{-AlOOH}$ . The transition is reversible and second-order, and thus the high-pressure state is probably unquenchable.