# Water and lower mantle phase transformations

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**Abstract**

The presence of water in many upper mantle minerals has been shown to have a large effect on their rheology in what is generally known as "hydrolytic weakening". A growing number of studies are finding that incorporating a water dependent rheology into global mantle convection models has a strong effect on global dynamics. However, while there is an abundance of experimental evidence showing that upper mantle minerals deformed under hydrous conditions are significantly weaker than when dry, there is no such experimental evidence for lower mantle minerals.

In this study we use DFT methods to calculate the partitioning of water between different sites in lower mantle minerals (bridgmanite, cubic and tetragonal calcium perovskite, ferropericlase and phase H) which allows us to speculate on the effects of water on lower mantle rheology.

We find that at typical lower mantle conditions water partitions preferentially into bridgmanite but with a mechanism that does not increase the vacancy concentration of bridgmanite and thus is unlikely to affect its rheology.

In cooler conditions, such as in a descending slab, water most prominently partitions into calcium perovskite. The presence of water in calcium perovskite has large effects on the preferred phase and can induce multiple phase transitions at varying depths of the lower mantle depending upon both water content and slab temperature. These transitions are likely to be seismically anomalous and could cause large seismic heterogeneity in descending slabs.
In conditions with large amounts of water ($> 5000$ ppm) water rich H phases can be formed but these are typically not favoured by the amount of water expected in the lower mantle.

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