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# Structure and properties of hydrous minerals from experiment and computation

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Within the ESF-EUROCORES program EuroMinScI / HydroMin we have begun to study the behaviour and role of hydrogen bonds in hydrous minerals by high pressure single crystal diffraction and by ultrasound spectroscopy at elevated pressure and temperature. We complement these experiments by density functional theory, DFT, based model calculations. After verification, the DFT models are used to interpret the measured behaviour on an atomistic level and to predict the behaviour at (P,T)-conditions beyond those accessible by experiment.

We show that quantum mechanical path integral molecular dynamics simulations are necessary to model the hydrogen dynamics in brucite, $Mg(OH)_2$. With linear response calculations we have shown that the experimentally determined very large pressure-induced frequency shift of the hydrogen stretching vibration in orthozoisite with respect to clinozoisite is not an artifact and that small structural changes can have an appreciable influence on the compression mechanism. DFT calculations correctly model the compression behaviour of diaspore and show that a symmetrisation of the hydrogen bond does not occur in the investigate pressure range ($P < 100$ GPa).

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