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Incorporation modes of hydrogen in ringwoodite: a DFT study

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Ringwoodite (γ-Mg_2SiO_4) is considered to be the most abundant mineral in the lower part of the transition zone (520 - 660 km depth) and can incorporate up to 2.7 wt % H_2O in the form of OH within its crystal structure. It has been shown that the presence of hydrogen can affect the physical and chemical properties of ringwoodite (e.g. electrical conductivity, seismic velocities) and therefore has important implications for the dynamics of the transition zone. However, the nature of water sites remains unclear and the origin of the very broad band between 3800 and 2400 cm^{-1} associated with OH in the FTIR spectra of ringwoodite is not yet explained.

The relative energies of hydrogen defects in ringwoodite have been determined by molecular modelling using the density functional theory (DFT). The pressure effect and the influence of a partial Mg-Si disorder have also been investigated. Results mainly suggest that hydrogen tends to associate with magnesium vacancies forming neutral defects. This hydration mechanism is in agreement with the interpretation of X-ray diffraction data (Kudoh et al., 2000, Phys. Chem. Minerals; Smyth et al., 2003, Am. Mineral.). Now, the modelling of infrared spectra of the most stable hydrogen defects should provide more constraints on the actual location(s) of hydrogen in natural samples and on the origin of the broad OH band observed.