

## Structure and density of H<sub>2</sub>O-rich Mg<sub>2</sub>SiO<sub>4</sub> melts at high pressure from *ab initio* simulations

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Water has a strong effect on silicate melt properties, yet its dissolution mechanism in depolymerized melts, typical for mantle composition, remains poorly understood. Here we report results of first-principles molecular dynamics simulations of hydrous Mg<sub>2</sub>SiO<sub>4</sub> melts with 6 wt.%, 16 wt.% and 27 wt.% H<sub>2</sub>O at pressure and temperature conditions relevant to the upper mantle and mantle transition zone. The results show that hydrogen not only bonds to network-forming cations Si, but also to network-modifying cation Mg which - nevertheless - remains the most important network modifier. There is no evidence to support the hypothesis inferred from experimental data that water may cause an increase in the melt polymerization for ultramafic magmas; the ratio of non-bridging oxygens per Si increases with the addition of the oxygen from H<sub>2</sub>O. The partial molar volume of water is independent on concentration in our simulations which allows us to examine the density of hydrous melt systematically. The critical water content - at which melts are neutrally buoyant compared to the surrounding mantle - is ~4 wt.% H<sub>2</sub>O for a pyrolite melt, much lower than the high water content (>10 wt.%) observed in petrological experiments and estimated thermodynamically for low-degree partial melts formed in the vicinity of the mantle transition zone.

Keywords: mantle transition zone, water in silicate melts