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A first-principles study of water in wadsleyite and ringwoodite: Implication for the 520 km discontinuity

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Abstract

The seismic discontinuity around 520 km is believed to be caused by the phase transition from wadsleyite to ringwoodite, the dominant minerals in the mantle transition zone (MTZ). Both wadsleyite and ringwoodite can contain more than 1.0 wt% water at MTZ's conditions, but it is not well known how water affects the wadsleyite-ringwoodite transition. Here we investigated water partitioning between wadsleyite and ringwoodite and the water effect on this phase boundary using first-principles calculations. Our results show that the presence of water will shift the phase boundary to higher pressures, and the width of the two-phase coexistence domain in the Mg_2SiO_4-H_2O system is insignificant at mid-MTZ conditions. For the $(Mg_{0.9}Fe_{0.1})_2SiO_4$ system, the incorporation of 1.0 wt% water can narrow the effective width of two-phase coexistence by two-thirds. Together with elastic data, we find that velocity and impedance contrasts are only mildly changed by the water partitioning. We suggest that compared to the anhydrous condition, the presence of 1.0 wt% water will increase velocity gradients across the wadsleyite-ringwoodite transition by threefold, enhancing the detectability of the 520 km discontinuity.

Keywords: Water partitioning, wadsleyite, ringwoodite, 520 km discontinuity, two-phase coexistence, mantle transition zone