Energy states of hydrogen in anhydrous mantle minerals

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The method of molecular dynamics (MD) is used to simulate positions and energy states of hydrogen in nominally anhydrous mantle minerals.From the results of the MD simulations, the small amounts of hydrogen in forsterite forms a Si-OH bond showing lack of the hydrogen bond. In wadsleyite, the O1-site is partially replaced by OH as a M3 site magnesium vacancy. In ringwoodite, hydrogen coordinate SiO4 tetrahedron oxygen as a magnesium vacancy. Decreasing O-O interatomic length with high pressure produces a strong hydrogen bond. A further important results is that hydrogen in the high pressure phase becomes more stable when such a hydrogen bond is made.