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Ab initio evaluation of point defects in bridgmanite under lower mantle conditions

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High-pressure experiments and theoretical calculations have indicated that bridgmanite hosts abundant point defects under lower mantle conditions potentially exerting a significant influence on mantle viscosity and conductivity[1-5]. In particular, the disappearance of oxygen vacancies in bridgmanite in the mid-lower mantle is suggested to cause a viscosity increase at ~1000 km depth[6]. Vacancies may also act as a sink for impurity elements (in the form of extrinsic point defects) and a potential reservoir for volatiles like noble gases, and so understanding how defect type and abundances change with depth in the mantle could be important for the transport and storage of such elements. To address this we performed *ab initio* calculations to investigate the various types of point defects in bridgmanite ($MgSiO_3$). The defect formation free energies and concentrations of Schottky defects, oxygen vacancy and cationic (Mg^{2+}) defects in bridgmanite were calculated under both MgO-rich and SiO_2-rich conditions at the PT conditions of the lower mantle. Among the three types of defects studied, the Schottky defect has the lowest concentration and the oxygen vacancy defect is the most populated, with concentrations up to 10^{-2} at low pressures. In agreement with recent experimental work[1] and previous theoretical studies[5] the concentration of these decrease strongly with depth. Nevertheless, a small population still exists even in deep lower mantle conditions. In addition, the strong temperature dependence of these vacancies means that the concentration in early forming mantle minerals would be much higher, and may still exist in any primordial domain as diffusion may not be fast enough to remove them depending on the grain size. This might have important implication for both the rheology and the storage of noble gases in these regions.

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