Water at the grain boundary interface: Insights from first-principles simulations

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Grain boundaries are important for technological and geophysical applications. Forsterite, the Mg end-member of the olivine system is a common rock-forming mineral in Earth's upper mantle. Its interaction with water is thought to play a key role in several geochemical processes, including water retention during planetary accretion. Atomistic insights about the incorporation mechanism of the hydrous component in various defect forms (such as point, linear, and planar (surface and interfacial)) and knowledge about their thermodynamic properties are therefore of great relevance from the geophysical viewpoint. We will focus on our recent work on hydrous grain boundaries in Mg_2SiO4. Our first-principles simulations of several tilt grain boundaries in Mg_2SiO_4 over the pressure range of 0 – 15 GPa suggest (i) greater energetic stability and negative excess volume (volume collapse) for the majority of hydrous grain boundaries relative to their anhydrous (dry) counterparts, (ii) dissociative adsorption as the main mechanism for water incorporation, and (iii) energetic preference of the hydrous component at the grain boundary interface over the bulk. Together, these results imply greater importance of grain boundaries in mantle processes.