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## First principle investigations on the water budget in olivine phases: Implications towards the behavior of hydrous mantle

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Several studies have already concluded the presence of 7-8 ocean equivalent water (OCE) in the mantle of earth, structurally occurring as  $H^+/OH^-$ . This can affect the seismic anomaly, mechanical strength, ionic diffusion, etc. of the mantle. The upper mantle is primarily composed of olivine, which first transforms to wadsleyite and then to ringwoodite at  $\sim 13$  and  $\sim 18$  GPa, respectively. Petrological and mineralogical experiments have demonstrated that H, occurring as point defects can act as a source of water in the upper mantle. Being the abundant mineral in upper mantle, it is very important to investigate the ability of olivine to act as a potential mineral phase to house water. Incorporation of water in mantle minerals has been a burning topic for many theoretical and experimental works. Even a trace amount of water in mineral structure can significantly alter their physical (e.g., elastic behaviour, seismic velocities, etc.) and chemical properties (e.g., ionic diffusion, electrical conductivity, etc.). FT-IR studies suggested that a rapid diffusion of  $H^+$  in olivine makes it a better candidate for point defects compared to larger and heavier  $OH^-$  ions. Karato & Jung (2003) showed that increment of H concentration in olivine decreases its strength. Later, Mao et al. (2008) and Panero et al. (2010) observed qualitatively similar trend in high pressure olivine polymorphs. They observed drastic reduction in selective elastic constants of  $C_{11}$  compared to  $C_{12}$  and  $C_{44}$  as H content increases in ringwoodite. Huang et al. (2005) found that temperature and water increases electrical conductivity in both the polymorphs. Yoshino et al. (2009) reported that a hike in temperature switches H-diffusion mechanism in olivine from proton conduction to small polaron conduction. The H diffusion in Fe-bearing olivine is experimentally shown to be dictated by (i) Proton-polaron (PP) mechanism and (ii) Proton-vacancy (PV) mechanism in  $<1$  GPa. The PV is found to be valid for incorporating more water in olivine compared to PP. However, the second method, despite being strongly anisotropic, allows a faster diffusion. Much of the existing studies deals with temperature and water content as the key physical factors in controlling proton diffusivity. The fact that most of these studies have not carried out in the exact pressure (p) and temperature (T) conditions of mantle of Earth demand further studies on the same. Present study involves the study of H diffusion in lattice structure of olivine and wadsleyite; their mechanical stability, physical and chemical properties under mantle  $p$ - $T$  conditions. Our results suggest a drop in seismic velocities in both olivine and wadsleyite phases. This can explain few outstanding geological events such as, weakening of upper mantle etc. This study will also provide a water budget in these mantle minerals. Therefore, the proposed research embarks on advancing theoretical understanding of hydrous mineral phases, which have a stability under extreme

thermo-mechanical conditions.