Hydrogen in Earth's Lowermost Mantle

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The lowermost mantle (D") is characterized by pronounced elastic anisotropy and elevated seismic attenuation. The presence of the post-perovskite (PPv) phase in the D" layer would contribute to these seismic observables, and therefore the influence of compositional variability on the physical properties of PPv should be explored to test mineralogical models of D" against the observed seismic structure. Here, we explore the influence of hydrogen on the physical properties of the PPv phase by first-principles calculations using density functional theory. The presence of hydrogen in the core-mantle boundary region, either as primordial H diffused from the liquid outer core or added by deeply subducted slabs, could potentially influence PPv physical properties and its phase stability. The OH-storage capacity of perovskite is likely much lower than PPv so the presence of OH could also influence the structure of D". In the upper mantle, even small amounts of OH at concentrations less than 0.1 wt% can influence elastic properties and lattice preferred orientation. To study the possible influence of hydrogen on the physical properties of PPv, we have determined a stable hydrogen defect structure for PPv and its associated elastic properties, thermal stability, and IR signature. We will present a comparison of the observed elastic properties of the D" region with the calculated elastic properties of hPPv, as well as calculated FTIR spectra for comparison to ongoing experiments using a new CO_2 laser-heating system and synchrotron-FTIR spectroscopy at the National Synchrotron Light Source.

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