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Hydride incorporation in Ti perovskites

William R Palfey, Sonjong Hwang, William A. Goddard, George R Rossman
California Institute of Technology

Abstract

Studies of nominally anhydrous minerals (NAMs) in the mantle have long focused on the hydroxyl group (OH⁻) as the primary hydrogen species of interest. However, titanate perovskites in the (Ca,Sr,Ba)TiO₃ composition range demonstrate the ability to incorporate high concentrations of an alternate hydrogen species – the hydride (H⁻) ion. Considering the high solubility of Ti in Ca perovskites like davemaoite (CaSiO₃), this presents the intriguing possibility of an unaccounted-for hydrogen reservoir in earth's mantle. Even so, questions remain surrounding hydride incorporation in mantle perovskites, including: How is H⁻ solubility constrained by pressure, temperature and fO₂? How would H⁻ partition between perovskite and Fe⁰ or FeH_x phases? Identifying and characterizing H⁻ in these materials, which carries unique technical challenges, will be critical for such future studies. Here, we present our efforts to characterize hydride-doped Ti perovskites primarily via infrared and ¹H nuclear magnetic resonance spectroscopies. These efforts encompass both naturally derived and synthetic materials, with particular focus on the SrTiO₃ and CaTiO₃ members of the titanate perovskite family. Density functional theory (DFT) calculations are crucial for interpreting spectroscopic measurements and provide a pathway to analyze hydride's possible coupling to the CaTiO₃ component of davemaoite. This work represents the first steps towards contextualizing the role of hydride in earth's mantle, and possibly the interiors of other planets.