

ヒドリドの特性を活かした組成、構造、機能制御

Design and Control of Structures and Functions using Characteristics of Hydride

Anions

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Oxyhydrides show novel properties associated with unique features of the hydride anion including lability, the lack of p orbitals in its outer most shell and high polarizability [1]. The observed properties include hydride conductivity in La_2LiHO_3 [2] heterogeneous catalysis in $\text{BaTi}(\text{O},\text{H})_3$ [3], and photochromism in LnO_xH_y [4]. $\text{BaTi}(\text{O},\text{H})_3$ is also shown to be a starting compound for topochemical anion-exchange reaction to yield a variety of mixed-anion compounds [5, 6]. Our recent study on SrVO_2H under pressure has revealed that the hydride anion is extremely flexible in size, with its compressibility twice as large as the oxide anion [7]. The size flexibility of H^- is then exploited to enable a novel anion order-disorder transition in LnHO (Figure 1) [8]; While LnHO ($\text{Ln} = \text{Sm}-\text{Er}$) adopts the anion-disordered fluorite structure, the anion ordering takes place for $\text{Ln} = \text{La}-\text{Nd}$, where H^- anions are expanded to form a larger HLn_4 tetrahedron. This expansion reduces the OLn_4 tetrahedral size and satisfies otherwise underbonded oxide anion. Furthermore, the anion order/disorder provides a significant influence on structures and hydride diffusion in the fluorite lattice [9, 10].

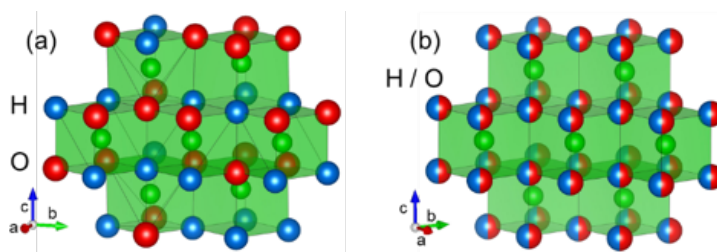


Figure 1 : Fluorite-type LnHO with (a) anion ordered and (b) anion disordered structure.

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