

論文 / 著書情報
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Title(English)	Hydride Ion Conduction in Anion-Excess Fluorite-Type Metal Hydrides
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Hydride ion (H^-) conduction in rare-earth (*RE*) hydride-based materials was investigated aiming at fast anion conduction at low temperature. Solid solutions of $\text{LaH}_3\text{-La}_2\text{O}_3$, $\text{LaH}_3\text{-CaH}_2$, and $\text{YH}_3\text{-MgH}_2$ were chosen as the host materials. These hydrides crystallized in anion-excess fluorite structure, and exhibited H^- conductivity ranging $10^{-7}\text{-}10^{-3} \text{ S cm}^{-1}$ at room temperature. High H^- conductivity of $\sim 1 \text{ mS cm}^{-1}$ at room temperature was observed in the samples with large amount of ‘excess’ H^- . Electronic conduction in *RE* hydrides was suppressed by partial substitution of oxygen and divalent metals (Ca^{2+} and Mg^{2+}) for H^- and RE^{3+} , respectively.

Fast H^- conductive nature of the anion-excess fluorite-type hydrides was understood from the characteristic crystal structure, i.e., the nearest neighbors of H^- in octahedral sites are not La^{3+} but H^- itself in tetrahedral sites. Molecular dynamics simulations revealed two types of mobile and immobile H^- and cooperative migration of H^- in $\text{LaH}_{3-2x}\text{O}_x$. This result suggests that the Coulombic repulsion between H^- ions drives cooperative migration and results in fast H^- conduction comparable to H^+ conduction in hydrated crystals. This finding will be a design principle for fast anion conductors.