Complex Hydrides for Multi-valent Ionic Conductors and Advanced Batteries

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Abstract

We have been developing a new materials science on hydrogen/hydrides to "fully-utilize" the diverse functionalities of hydrogen in materials. One of the research targets is a series of complex hydrides exhibiting various energy-related properties. So far, we have reported the systematic studies on Li super-ionic conduction and all-solid-state lithium-ion battery using an optimized solid-solution phase of $LiCB_9H_{10}$/$LiCB_{11}H_{12}$. A detailed MD simulation on the cation conductivity was also reported on the related system.

In addition to monovalent cations of Li^+ and Na^+, our research endeavors encompass divalent cations, specifically Mg^{2+}, Zn^{2+}, and Ca^{2+}. Focusing on the development of a robust and efficient Ca^{2+} liquid electrolyte for Ca metal batteries, we have developed on a novel complex hydride, $Ca(CB_{11}H_{12})_2$. The $Ca(CB_{11}H_{12})_2$ electrolyte exhibits outstanding performances of reductive/oxidative stability and high conductivity, thereby enabling durable battery operation. Recently, a genetic algorithm method combined with ab initio kinetics and molecular dynamics simulations have succeeded in exploring the ionic conductivity trends of complex hydrides.

Moreover, we are constructing a "Dynamic Database of Solid-State Electrolyte (DDSE, >2000 materials including the complex hydrides)" that will be a new avenue to understand the structure-performance relationships and find out new design guidelines: See; F. Yang, E. Santos, X. Jia, R. Sato, K. Kisu, Y. Hashimoto, S. Orimo, H. Li, Nano Mater. Sci., 6 (2024) 256.