# 錯体水素化物中の一価および多価陽イオンの高速伝導現象とその電池応用 ー“ハイドロジェノミクス”の視点からー

# Fast-ionic conduction of mono-/di-valent cations and advanced battery application of complex hydrides ー Viewpoints from “HYDROGENOMICS” ー

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Hydrogen in materials exhibits a wide range of concentration, high mobility, quantum nature, and superior chemical reactivity. All these features of hydrogen originate from its bonding and size flexibilities. The goal of the MEXT (Ministry of Education, Culture, Sports, Science and Technology, Japan) project is to develop a new materials science on hydrogen and hydrides as a guideline to “fully utilize” the diverse functionalities of hydrogen in materials [1].

One of the research targets of this project is a series of complex hydrides exhibiting various energy-related properties [2]. So far, we have reported the systematic studies on lithium super-ionic conduction and all-solid-state lithium-ion battery using an optimized solid-solution phase of complex hydrides $LiCB_9H_{10}$/$LiCB_{11}H_{12}$ [3]. A detailed molecular dynamics simulation on the order-disorder phase-transition behavior, re-orientational anion motion, and cation conductivity was recently reported on the related system [4].

In addition to the mono-valent cations, lithium and sodium [5], we have been also focusing on the di-valent cations, magnesium [6] and calcium. We have been developing a highly stable and efficient Ca electrolyte composed of a new complex hydride $Ca(CB_{11}H_{12})_2$ for RT-operating calcium-ion battery [7]. This $Ca(CB_{11}H_{12})_2$ electrolyte exhibits excellent electrochemical performances; that is, the high conductivity, wide potential window, and reversible Ca plating/stripping with high Coulombic efficiency.

Furthermore, we are studying complex hydrides with pseudo-rotational anion motion, such as $Li_5MoH_{11}$ with $[MoH_9]^{3-}$, as new candidates of super-ionic conductors of various cations [8].

**References**

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