

Title **Complex Hydrides for Multi-valent Ionic Conductors and Advanced Batteries****Speaker** Prof. Shin-ichi ORIMO ^{1,2,3,4}

1 Advanced Institute for Materials Research (WPI-AIMR), Tohoku University, Japan

2 Institute for Materials Research, Tohoku University, Japan

3 Institute of Materials Structure Science (IMSS), KEK, Japan

4 Center for Energy Systems Design, I²CNER, Kyushu University, Japan**Time&
Date**

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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 LiCB₉H₁₀/LiCB₁₁H₁₂. 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 Mg²⁺, Zn²⁺, and Ca²⁺. Focusing on the development of a robust and efficient Ca²⁺ liquid electrolyte for Ca metal batteries, we have developed on a novel complex hydride, Ca(CB₁₁H₁₂)₂. The Ca(CB₁₁H₁₂)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.

About the Speaker

Shin-ichi ORIMO received his Ph.D. in 1995. He was a JSPS research fellow, a research associate in Hiroshima University, and a guest researcher in Max-Planck Institute for Metal Research awarded by Humboldt Fellowship and MEXT Fellowship. So far, he received "Metals Meritorious Award", "The Commendation for Science and Technology, the Minister of MEXT", "Science of Hydrogen & Energy Award", "Honda Frontier Award". He has been the Director of WPI-AIMR (World Premier International Research Center Initiative - Advanced Institute of Materials Research), Tohoku University, also the PL of Grant-in-Aid for Scientific Research on Innovative Areas "Hydrogenomics", and the TL of JST-GteX program “Innovative Hydrogen Storage”.

Registration https://zoom.us/webinar/register/WN_RkETIOpaSz-ZCynuj6r7PQ**Host** Prof. Masanobu Kubota

Contact I²CNER · Q-PIT Office of Research Support Services,
Research Support and Public Relations
TEL: +81 92 802-6935
Email: iq-kenkyu@jimu.kyushu-u.ac.jp

