


Hydrogen ion ceramics

	Principal Investigator	Kyoto University, Graduate School of Engineering, Professor	
		KAGEYAMA Hiroshi	Researcher Number: 40302640
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Purpose and Background of the Research

●Outline of the Research

This project aims at establishing a new field of hydrogen-involved ceramics by developing new materials and synthesis strategies involving  $H^+$  and  $H^-$  ions, and exploring novel functions. This research will accelerate the realization of hydrogen economy by game-changing synthesis of hydrogen-based materials. It is clear that the realization of hydrogen society is an urgent necessity if the world is to depart from its dependence on fossil fuels. While technological development related to hydrogen energy is active around the world, there is significant room for development in the creation of materials that utilize hydrogen. In this project, we will provide comprehensive understanding on the hydrogen in ceramics materials, essential for hydrogen economy.

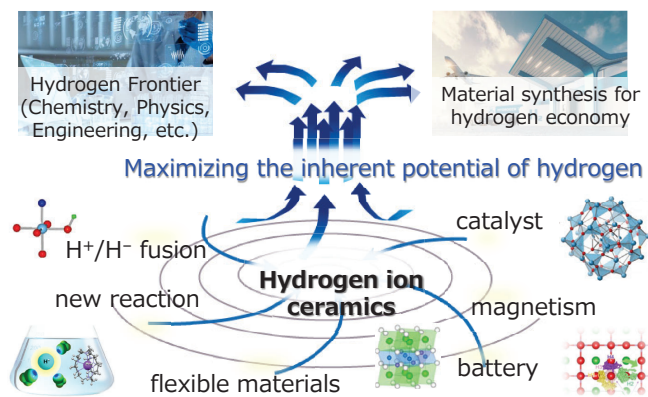


Figure 1. Hydrogen ion ceramics

Hydrogen science faces three challenges. First, proton chemistry is saturated in terms of both material synthesis and functionalities, in contrast to biochemistry and organic chemistry, where protons are responsible for a variety of reactions and functions. There is still room for breaking the limit of proton chemistry in ceramics. Second, as for hydrides, the variety of materials are very limited. One of the major reasons for this is that the synthesis method is limited to solid-phase reactions, making it difficult to control the shape, size, and exposed surface of the particles, which is essential for the design of functional materials. Finally, development of functionalities derived from the coexistence of protons and hydrides is unexplored in ceramic materials. On the other hand, in organic chemistry, molecules in which  $H^+$  and  $H^-$  coexist have been developed and are contributing greatly to the field of catalysis. This is another unexplored area of hydrogen-based ceramics.

Prof. Kageyama, the Principal Investigator of this project, is a world leading researcher in mixed anion compounds (A review, Nat. Commun. 2018), and has been involved in their synthesis, the development of synthetic approach, and the development of innovative functions. For example, he found introducing hydride can activate an oxide, thereby providing functional properties as an efficient and stable catalyst (Figure 2). In recent years, he has also discovered a new method for reducing oxides by electrochemical protonation followed by dehydration (J. Am. Chem. Soc. 2021). Based on these findings, this project will bring a breakthrough in the field of functional hydrogen-based ceramic materials by focusing on the characteristics of hydrogen and developing synthesis methods.

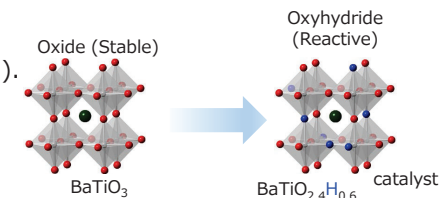


Figure 2. Inclusion of hydride ions activates an oxide (Nat. Mater. 2012, J. Am. Chem. Soc. 2017)

Expected Research Achievements

In light of the current situation, this project will address three main themes to maximize the inherent potential of hydrogen: (1) "Beyond the limitations of proton", (2) "Advancing hydride research to a new phase", and (3) "proton-hydride fusion". For (1), we will develop catalysts based on positively charged clusters (Figure 3) and new materials using the recently developed reduction method (Figure 4). For (2), we will develop synthetic methods for hydride materials and new functions utilizing the high polarizability of hydride anions. For (3), we will synthesize new ceramic materials in which protons and hydrides coexist to develop novel functions that are difficult to achieve with organic materials. We also aim to observe non-trivial hydrogen ion conduction process, as shown in Figure 5. Through these studies, we will provide a comprehensive understanding of hydrogen in ceramics, which has been so far separately studied.

An interdisciplinary group consisting of nine researchers is organized to create materials and explore the functions of hydrogen-based ceramics. Hiroshi Kageyama: solid state chemistry, Hiroshi Takatsu: solid state physics, Cedric Tassel: structural chemistry, Daichi Kato: mixed anion chemistry (Kyoto Univ.), Susumu Fujii: computational physics (Osaka Univ.), Hitoshi Takamura: solid state ionics (Tohoku Univ.), Yasuhide Inokuma: organic synthesis (Hokkaido Univ.), Sayaka Uchida: catalysis chemistry (Univ. Tokyo), Shunsuke Kobayashi: electron microscopy (JFCC).

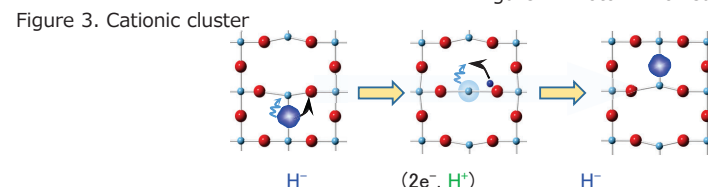
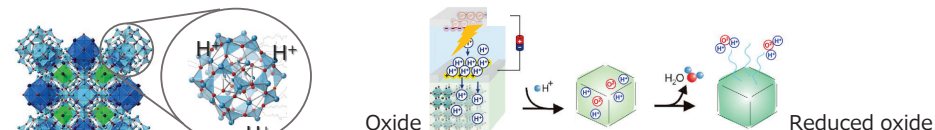


Figure 5 Non-trivial hydrogen ion conduction coupled with electron transfer