



Title of Project : **HYDROGENOMICS: Creation of Innovative Materials, Devices, and Reaction Processes using Higher-Order Hydrogen Functions**

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【Purpose of the Research Project】

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. (Fig. 1)

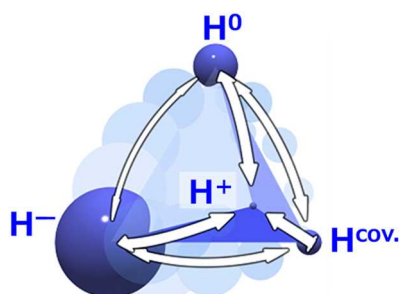


Fig. 1 Hydrogen diagram illustrating the bonding and size flexibility of hydrogen in materials; the spheres located at each vertex represent proton (H^+), hydride ion (H^-), covalently bonded hydrogen ($H^{cov.}$) and neutral hydrogen (H^0). The sizes of hydrogen are also drastically changed according to the bonding states.

The purpose of this project is to develop a new materials science of hydrogen / hydrides (hereafter referred to as “Hydrogenomics”, i.e., hydrogenomics) as a guideline to “fully utilize” the diverse functionalities of hydrogen in materials.

【Content of the Research Project】

The project will focus on the four most important functionalities of hydrogen originated from its bonding and size flexibilities (hereafter, referred to as “hydrogen functions”); i.e., “high densification ability (A01)”, “interfacial localizability (A02)”, “fast migration ability (A03)” and “high activation ability (A04)”. Then the project will merge them to induce unprecedented “higher-order hydrogen functions (synergistic effect between its individual hydrogen functions)” with the support of “advanced analysis and simulation techniques (A05)”, which will also be developed within this project to capture the hydrogen functions more accurately than ever done before. (Fig. 2)

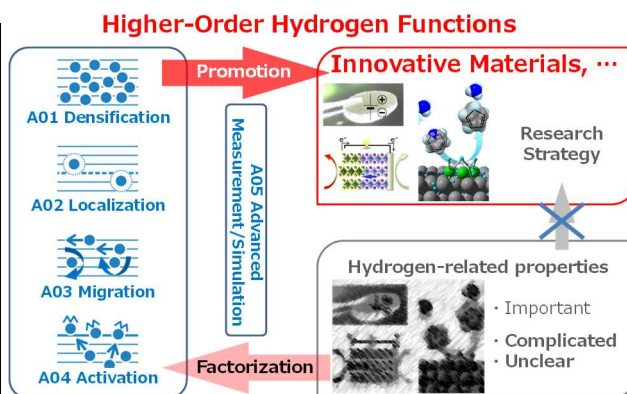


Fig. 2 Strategy of Hydrogenomics.

【Expected Research Achievements and Scientific Significance】

- Synthesis of hydride superconductors and super-ionic conductors.
- Proof-of-principle for hydride electronics, and enhancement of photovoltaics and high-strength steel properties.
- Production of advanced energy generation / storage and new-concept devices using hydrogen-electron coupling and hydride super-ionic conductors.
- Performing new material-conversion processes using hydrogen.
- Clarification of the mechanism determining the hydrogen functions and realization of high-accuracy analysis based on hydrogen data-assimilation technique.
- Promotion of young researchers training and social implementation, and formation of international network, in the related research field.

【Key Words】

Hydrogenomics, Higher-order hydrogen functions

【Term of Project】 FY2018-2022

【Budget Allocation】 1,135,000 Thousand Yen

【Homepage Address and Other Contact Information】

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