【Grant-in-Aid for Transformative Research Areas（A）】

Deuterium Science 2. 0

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Project Information	Project Number : 26A403　　Project Period (FY) : 2026-2030 Keywords : Deuterium, Deuterated Materials, Deuterated Drugs, Isotope Effect

Purpose and Background of the Research

●Outline of the Research

Deuterium (^2H, D) is a stable isotope of hydrogen. Deuterium is one of the most familiar isotopes, present in small amounts in water in nature. Unlike tritium (^3H), deuterium is non-radioactive. Although deuterium-labelled compounds generally exhibit chemical properties similar to those of protium analogs, their physical properties are significantly different in some cases. By leveraging these pronounced isotope effects, deuterium labeling has recently enabled the development of pharmaceuticals with improved safety and metabolic stability (deuterated drugs), as well as organic light-emitting diode (OLED) materials with enhanced emission efficiency and durability (deuterated OLEDs). As a result, the design and application of deuterated compounds have become increasingly active worldwide. Because hydrogen is ubiquitous in most molecules, the rational replacement of hydrogen with deuterium ("deuterium switch") is expected to enable the design of materials that surpass conventional performance limits. From this perspective, isotopes are regarded as a new guiding principle for molecular design. In this context, we have previously initiated a collaborative project named "Deuterium Science" between theory and experiment, supported by the MEXT grant-in-aid for transformative transformative research areas(B) 2020-2022FY. In order to further expand this scheme, this transformative research area "Deuterium Science 2.0" aims to establish a new interdisciplinary field, "Deuterium Science," by integrating informatics, theoretical science, and experimental science (chemistry and biology) to systematically understand the properties of deuterium labeled materials and to explore their applications for developing innovative materials beyond conventional technological limits (Fig. 1).

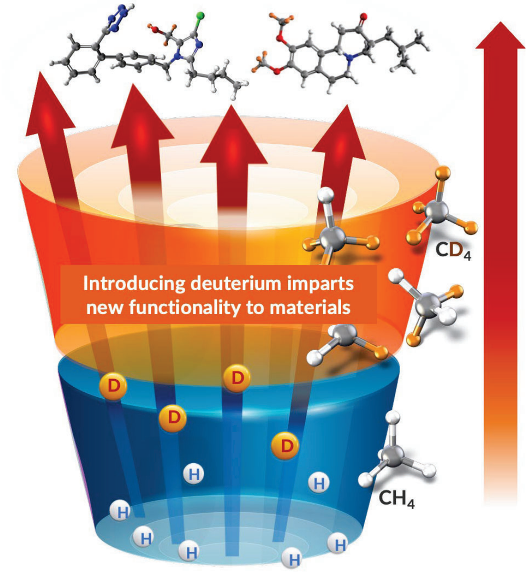

Figure 1. Overview of Research Area

Expected Research Achievements

This research area integrates four domains: A01 Selection (Applied Informatics), A02 Understanding (Quantum Mechanics), A03 Synthesis (Synthetic Chemistry), and A04 Measurement (Advanced Measurement, Fig. 2). Through collaboration across these domains, we aim to elucidate properties of deuterated materials that have been difficult to predict using conventional approaches and to establish a new scientific framework: Deuterium Science. Collaborative research within this program will drive the development of innovative materials and technologies that contribute to a sustainable society. Possible examples includes safer pharmaceuticals, high-performance luminescent materials, and sensitive molecular probes.

A01 Selection (Design & Prediction, Informatics, AI)

The team A01 integrates data on deuterated materials to establish new methodologies for property prediction and molecular design. Databases will be established from the outputs of teams A02–A04 and data-driven approaches will be developed for understanding, prediction, and validation.

A02 Understanding (Quantum Mechanics, Theoretical Chemistry)

The team A02 establishes theoretical foundations for understanding deuterium effects. New hybrid methods of non–Born–Oppenheimer (non-BO) calculations with realistic computational methods (e.g., QM/MM, CPLB) will be developed. Isotope effects on reactivity, vibrations, and excited states will be examined.

A03 Synthesis (Synthetic Chemistry, Synthetic Biology)

The team A03 develops practical synthetic methods of deuterated materials. Based on bottom-up and top-down approaches, catalytic H/D exchange will be explored and, through collaboration, previously unexplored deuterated biomolecules will be produced.

A04 Measurement (Advanced Measurement, Functional Evaluation)

The team A04 acquires data on deuterated materials and evaluates isotope effects on material properties using advanced measurement techniques. Isotope effects in quantum materials and biological systems will be analyzed.

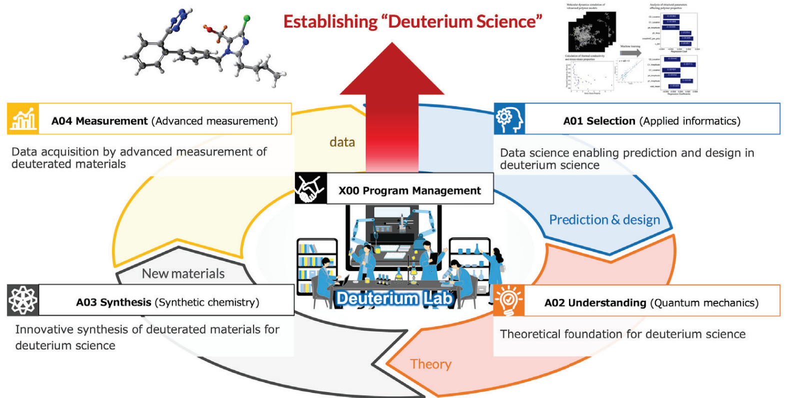

Figure 2. Research framework

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