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

Stochasticity-Driven Chemistry: Toward the Principle and Functions of Fluctuation-Powered Chemical Engines

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Project Information	Project Number : 26B202　Project Period (FY) : 2026-2028 Keywords : Non-equilibrium systems, Molecular motor, Metal organic framework, Fluctuations, Structural phase transition

Purpose and Background of the Research

●Outline of the Research

"Stochastic-Driven Chemistry" aims to establish the fundamental principles of chemical engines that harness stochastic fluctuations, such as random molecular motion and stochastic chemical reactions. To achieve this, we develop the energetics of stochastic fluctuations and elucidate the design principle of molecular motors.

Furthermore, by utilizing porous frameworks that combine structural regularity with flexibility, we construct a porous chemical engine—**STochastic Engine by Active Macroporous framework (STEAM)**—capable of energy extraction, storage, and conversion. This STEAM chemical engine will transform the laws of thermodynamics and opens a new field spanning non-equilibrium physics and chemical engineering.

●Research background

Many natural systems exist far from thermal equilibrium due to continuous energy input. In particular, molecular motors convert chemical energy into directed motion, functioning as nanoscale chemical engines and suggesting mechanisms that harness stochastic fluctuations as an energy source. In this context, we focus on metal–organic frameworks (MOFs), porous materials with high surface area. Soft MOFs exhibit "gate-opening adsorption," a structural phase transition in which guest molecules are taken up or released in response to external pressure. The shared features of molecular motors and Soft MOFs motivates us to construct nanoscale engines capable of energy extraction from stochastic fluctuations.

●Goal of research project

We elucidate the design principle shared by two seemingly distinct systems, molecular motors and Soft MOFs, and construct a chemically powered molecular engine, STEAM (Fig.1). Through this approach, we establish chemical energetics, in which stochastic fluctuations in motion and chemical reactions serve as a fundamental energy source.

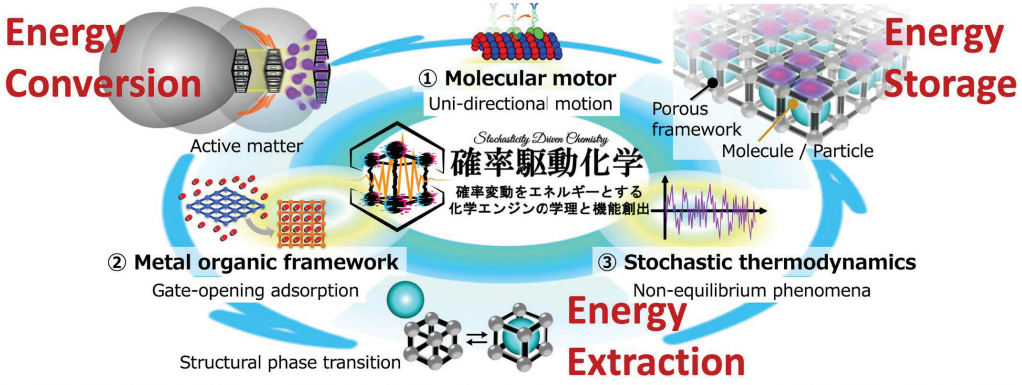

Figure 1. The research overview of the project "Stochasticity-driven chemistry"

●STEAM : Stochastic Engine by Active Macroporous framework

Soft MOFs organize the arrangement of adsorbed molecules while not completely constraining their motion, thereby regulating chemical reactions under fluctuating conditions. We exploit the stochastic nature of molecular motion and structural dynamics to construct a stochastic-driven porous engine, STEAM, capable of extracting and storing chemical energy and converting it into mechanical energy.

STEAM is a porous soft-matter-based framework that exhibits two states depending on the presence or absence of adsorbed particles (Fig. 2).

The realization of STEAM will contribute to the development of active matter that efficiently utilize fluctuations, thereby offering broad scientific impact.

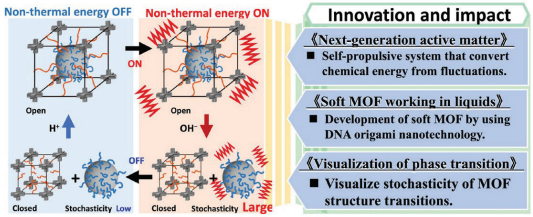

Figure 2 The concept of STEAM chemical engine

Expected Research Achievements

●Summary of the research projects

Four research teams integrate biophysics, non-equilibrium physics, chemical engineering, and synthetic chemistry (Fig. 3).

Project A01: Maeda group develops the energetics for chemical energy conversion from stochastic fluctuations within STEAM.

Project A02: Harashima group aims to enhance the performance of DNA-based artificial molecular motors through rational rail design and to utilize DNA origami to construct STEAM.

Project B01: Watanabe group investigates the gate-opening adsorption mechanism of Soft MOFs and STEAM, treating it as a stochastic phase transition at the single-domain level.

Project B02: Kusaka group controls the structural properties of Soft MOFs and STEAM to demonstrate cooperative structural phase transitions coupled with cascade-like molecular transformations within the frameworks.

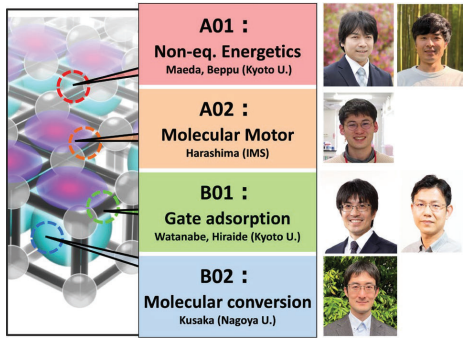

Figure 3 Research teams in the project

●Coordination for opening a new field

To ensure smooth progress of the research area and strong collaboration among projects, the coordinating group will be organized into three working groups: Transformation WG, Theory WG, and Synthesis WG (Fig. 4).

The outcomes of this research will extend beyond biophysical studies of molecular motors to fields such as CO_2 adsorption materials, photochemical reactions, thereby opening up emerging interdisciplinary areas across physics, chemistry, and life sciences.

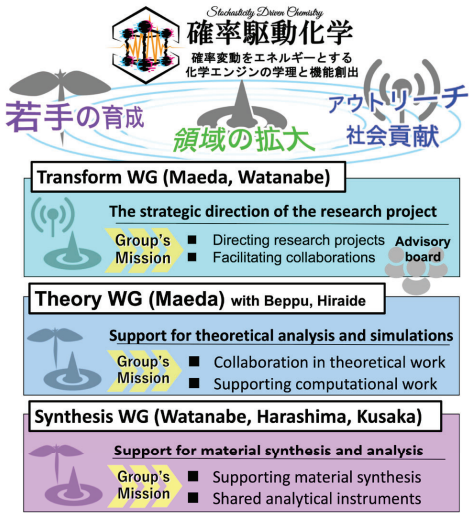

Figure 4 Project management and organization

Website(s)	Website https://steam.cheme.kyoto-u.ac.jp/	X https://x.com/stochastic_chem