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

Study of the Reaction Driving Force for Efficient Carbon Recycling （Reaction Driving)

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Research Area Information	Number of Research Area : 22B207　Project Period (FY) : 2022-2024 Keywords : catalysis, nanomaterials, carbon recycle, membranes

Purpose and Background of the Research

●Outline of the Research

Reducing carbon dioxide (CO_2) emitted from social activities into useful chemical substances is essential to realize a carbon-neutral society. However, the present methods require a high concentration of CO_2 at high temperatures, such as factory exhaust. The three barriers must be overcome to realize CO_2 reduction at room temperature under ambient pressure with high selectivity: (1) the catalytic activity barrier (Sabatier limit), (2) the selectivity barrier (conversion-selectivity interaction), and (3) the mass transport barrier (Robeson limit). This research area focuses on the driving forces that transcend each of these barriers (Figure 1).

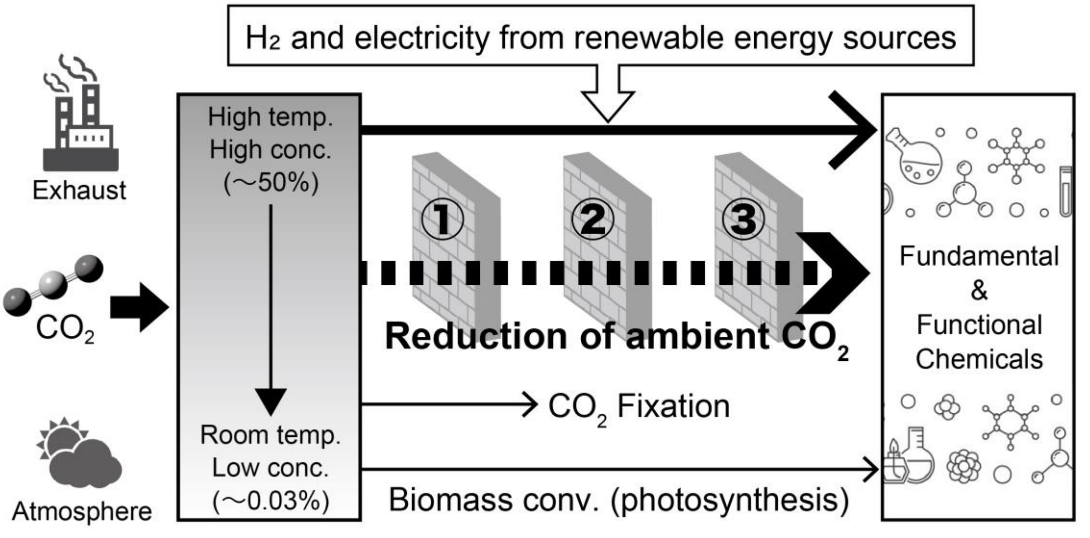

Figure 1: The goal of this research area: three barriers to overcome

●Research Approach

Barriers (1) to (3) are due to trade-offs among multiple chemical processes (chemical reactions and mass transfer), standing in the way not only of CO_2 reduction but also of various other conversion processes. However, it has been theoretically demonstrated that the barrier (1), for example, cannot be overcome by simply extending the catalyst design with conventional active sites such as metal/inorganic solid surfaces or metal complexes. This research area aims to solve these problems by going back to basic science.

Ultra-small metal/alloy particles (subnanoparticles) consisting of a few to several dozen atoms are promising materials, having a dynamically moving active site for catalytic CO_2 reduction at low temperatures. The CO_2 reduction driven at room temperature and pressure is expected by introducing subnanoparticles into the inside nanospace of a CO_2-concentrating zeolite (a type of boiling stone) and employing selective mass transport membranes that effectively expel water produced by the reaction from the active site.

●Overview of the research organization (Fig. 2)

Imaoka (A01) conducts screening of metal/alloy subnanoparticles. The promising candidate catalysts will be introduced into the zeolite synthesized by Oda (A02). Because this zeolite can internally concentrate CO_2 more than 200 times, the pressure required for the reaction is expected to be significantly reduced, resulting in a CO_2 reduction at ambient temperature and pressure.

A selective mass transport membrane that delivers only CO_2 and hydrogen to the active site and effectively removes the produced water from the active site is required. Saito (A03) fabricates this transport membrane.

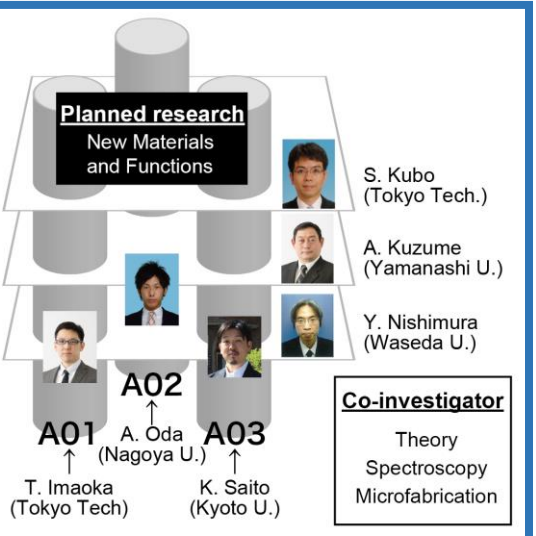

Figure 2: Research organization

Expected Research Achievements

●Research Goals

The outcome expected from this research area is a catalytic system that can selectively convert CO_2 into beneficial chemicals at ambient temperature and pressure. However, as mentioned above, it has been theoretically proven that it is impossible to achieve this goal by simply improving existing catalysts and systems. How can this be overcome? In this research area, we would like to demonstrate that removing the assumption of "invariant active sites that do not change," which has been the premise of catalytic science to date, will lead to this revolutionary material conversion (Fig. 3).

●Toward the Formation of an Interdisciplinary Field

The researchers currently belonging to this research area cover a wide range of chemistry and materials science fields, including organic, inorganic, and coordination chemistry, in addition to electrochemistry, catalysis, surface science, computational chemistry, nanoscience, spectroscopy, and green chemistry (Fig. 4). To reach the ultimate goal of realizing a carbon-neutral society, we will conduct research activities in this area toward creating the science of "reaction-driving" while deepening exchanges with researchers in other fields.

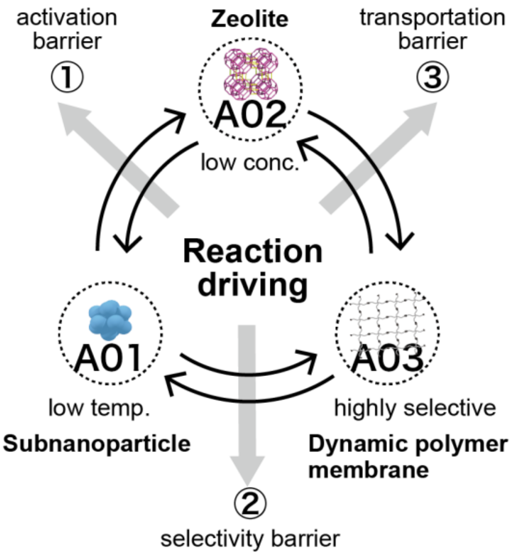

Figure 3 Creation of new science that drives efficient CO_2 reduction reactions.

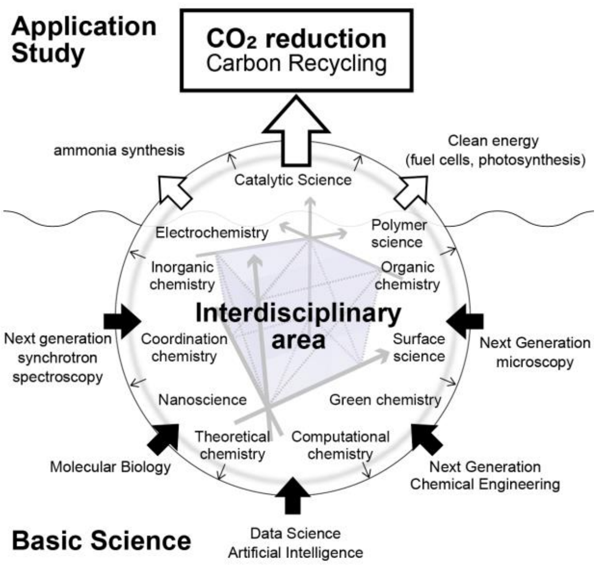

Figure 4 Formation of the interdisciplinary area around the "reaction-driving" science.

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