【International Leading Research】

Operando-analysis-based design of heterogeneous catalysts for carbon neutrality

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Project Information	Project Number : 23K20034 Project Period (FY) : 2023-2029 Keywords : Carbon neutrality, carbon dioxide, biomass, catalyst, *operando* analysis

Purpose and Significance of the Research

Global warming has been caused mainly by carbon dioxide as a result of the utilization of fossil resources. De-fossil resources are essential for achieving carbon neutrality (CN). This project aims to facilitate CN by developing the concept depicted in Fig. 1, with an emphasis on shifting from fossil fuels to renewable ones such as carbon dioxide and biomass. Such changes require drastic technological progress for achieving the necessary chemical transformations at the large scales required to make an impact towards CN. In contrast to our current petrochemical technology mainly relies on "oxidation" reactions for introducing oxygen functionality into molecules, the utilization of CO_2 and biomass-derived feedstocks necessitates the partial or complete removal of oxygen atom(s) via "reduction" reactions, thereby requiring orthogonal chemical approaches to be developed for achieving CN.

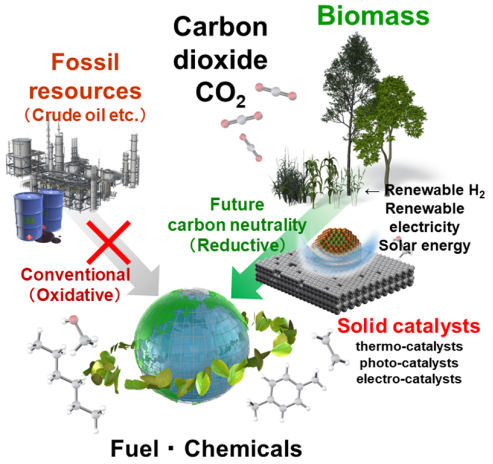

Fig. 1 Concept of this project toward carbon neutrality (CN)

To tackle this grand challenge, it is critical to develop new catalysts that increase efficiency of chemical processes relying on carbon dioxide and biomass-related feedstocks, by conducting reactions with higher selectivity and lower energy input. This project leverages talent around the world in part because CN is a global target, and it emphasizes the development of early-career researchers, who will be key players for ultimately achieving CN by the goal of 2050. This project, therefore, aims to train young researchers to become internationally renowned experts through overseas collaborations in top-level groups in the area of "catalyst development".

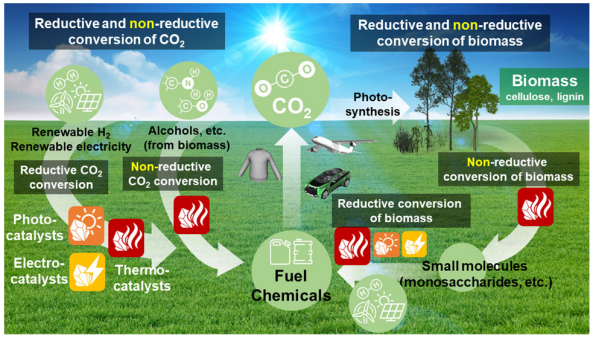

Fig. 2 Reductive and non-reductive conversion of carbon dioxide and biomass

The purpose of this project is the development of heterogeneous catalysts for four categories of catalytic reactions, *i.e.*, reductive and non-reductive conversion of carbon dioxide, and reductive and non-reductive conversion of biomass (Fig. 2).

Organization of the Project Team

The principal investigator (PI) and co-investigators (Co-I) leverage their unique expertise in heterogeneous catalysis for the conversion of carbon dioxide and biomass-derived compounds, and the characterization of such catalysts. They are coming together in this project and will provide training for early-career researchers and/or PhD candidates in top-level research groups throughout Europe, the U.S., and Asia, via international collaborations (Fig. 3), which are aimed at accelerating the realization of CN through catalyst development.

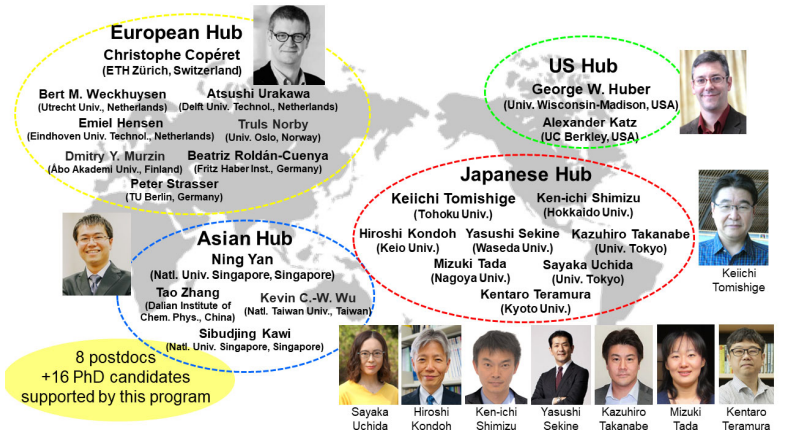

Fig. 3 Members of the project

Plan for Fostering Early-career Researchers

Catalyst development is essential for the realization of CN, and expertise in the field of catalyst development has undoubtedly become more important than ever before. An important feature of catalysts is the changes of structures and states of catalytically active sites in the working state involving heat, photo-irradiation, electric field gradients, the co-presence of substrates, *etc.* Therefore, cutting-edge "*operando*" spectroscopies will be used to characterize the catalysts developed by the PI or Co-Is in the working states, and the resulting data will inform further development of catalysts with even higher level of performance. In this project, eight early-career researchers and sixteen PhD candidates will be sent to overseas laboratories managed by top-level researchers who have expertise in unique characterization techniques and skills in the area of catalysis and reaction engineering (Fig. 4). These experiences will facilitate growth in the area of catalyst development for CN.

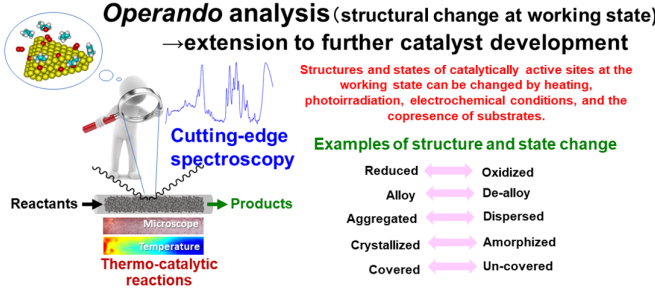

Fig. 4 Image of *operando* analysis of catalysts at working state

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