【Grant-in-Aid for Scientific Research (S)】

Broad Section D

Title of Project : Design and development of novel active sites on heterogeneous catalysts using direct interaction of molecules with solid surfaces

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Keyword : Catalyst function, biomass, CO_2

【Purpose and Background of the Research】

Lots of chemicals have been produced from petroleum. From the viewpoint of CO_2 emission and limitation of petroleum, the technologies for the conversion of biomass and CO_2 are necessary for the sustainable society. Heterogeneous catalysts are more promising in terms of the catalyst separation and reusability. At the same time, the increase of the total energy efficiency can be enhanced by the replacement of present multi-step processes with one-pot conversion using heterogeneous catalysts, which is also connected to the decrease of CO_2 emission. The purpose of this research is to develop heterogeneous catalysts for the efficient conversion of biomass and CO_2 and to propose the design and preparation methods of catalytically active sites as a key of the catalyst development.

【Research Methods】

The aim of this study is to make the catalytically active site with high performance through the synergy of modifiers such as molecules or clusters and solid surfaces by the direct interaction. A typical example of the preparation of heterogenous catalyst is shown in Figure 1 (a).

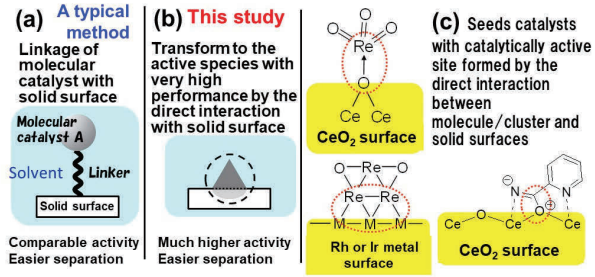

Figure 1. Preparation method of heterogeneous catalysts (a), (b) and seed catalysts prepared by the direct interaction between modifiers with solid surfaces (c)

In this study, we challenge to transform to the highly active species by the direct interaction with solid surfaces (Figure 1 (b)). The combination giving strong synergy is very limited. Broad and careful surveys have been essential in order to find an effective combination. In this study, the details of our seed catalysts are investigated using near-ambient pressure X-ray photoelectron spectroscopy combined with various characterization methods and computational chemistry.

【Expected Research Achievements and Scientific Significance】

Seed catalysts are isolated ReO_x species on CeO_2 surface for deoxydehydration, ReO_x clusters on Rh or Ir surfaces for C-O hydrogenolysis, and CeO_2+2-cyanopyridine for the conversion of CO_2+alcohols to organic carbonates (Figure 1(c)). These catalysts showed high performance in the production of value-added chemicals from biomass and CO_2, however, a problem is the usage of noble metals or complicated molecules. For the substitution with cheaper and more abundant metals or simpler molecules, different counter components can be found effectively on the basis of the results of the analyses of the seed catalysts. The development of catalysts without containing noble metals and complicated molecules can enhance the feasibility of the process remarkably.

【Publications Relevant to the Project】

・Transformation of Sugars to Chiral Polyols over a Heterogeneous Catalyst, M. Tamura, K. Tomishige, et al., Angew. Chem. Int. Ed., 57, 8058-8062 (2018)
・Self-Assembled Hybrid Metal Oxide Base Catalysts Prepared by Simply Mixing with Organic Modifiers, M. Tamura, K. Tomishige, et al., Nature Commun., 6, 8580 (2015)

【Term of Project】 FY2018-2022

【Budget Allocation】 146,900 Thousand Yen

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