

【Grant-in-Aid for Specially Promoted Research】

Next-generation catalytic reactions driven by activation of hydrogen



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Purpose and Background of the Research

● Outline of the Research

Reduction of CO₂ and biomass-related compounds becomes more important because these reactions will contribute to the realization of carbon recycling and carbon neutrality. Hydrogen will be efficiently produced by renewable methods such as light or electricity in the near future, suggesting the arrival of hydrogen society. The purpose of this research is the development of catalytic systems for selective reduction of CO₂ and biomass-related compounds using H₂ as a reductant to useful fuels and chemicals even under lower hydrogen pressure and/or lower reaction temperature than conventional methods.

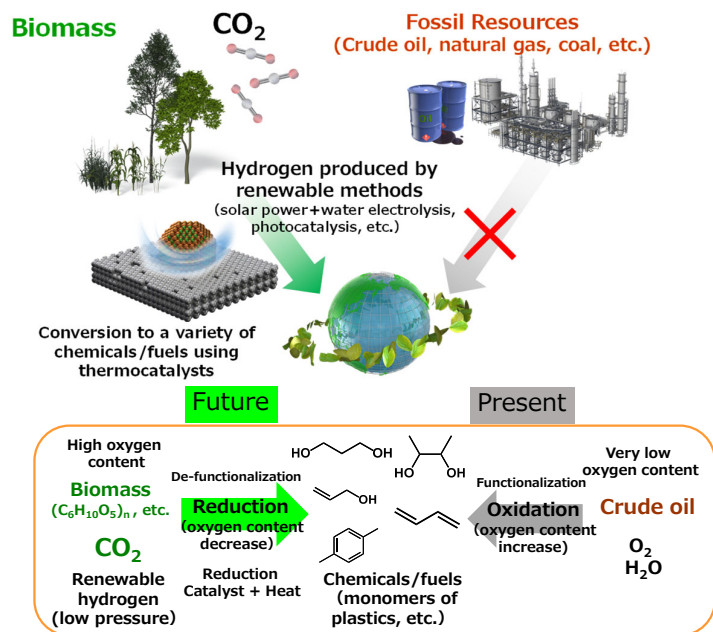


Figure 1. Carbon recycling, carbon neutrality, and de-fossil resources driven by reduction of CO₂ and biomass-related compounds

● Utilization of our catalysts for hydrodeoxygenation of biomass-related compounds

The PI has been developing effective catalysts for the hydrodeoxygenation (the decrease of oxygen content by the reduction with hydrogen) of biomass-related compounds such as glycerol and erythritol. This research utilizes our developed catalysts (e.g., Iridium nanoparticles modified with Rhenium oxide clusters, isolated Re species attached on CeO₂ surfaces, etc.).

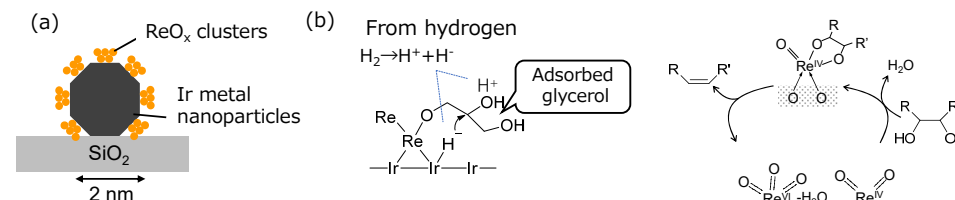


Figure 2. Models of Iridium metal nanoparticles modified with Rhenium oxide clusters (a) and metal-oxide interface as a catalytically active site for C-O hydrogenolysis (b)

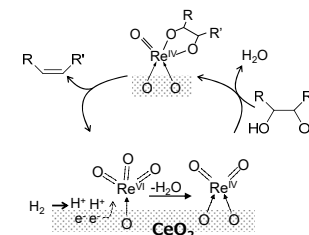


Figure 3. Deoxygenation of vicinal OH groups over isolated Rhenium species attached on CeO₂ surface (H₂: reducing agent)

● H₂: Cheap and useful reducing agent

Hydrogen has been produced by the reaction of fossil resources (mainly natural gas) with steam, and highly pressurized hydrogen can be supplied on the basis of the synthesis reaction conditions. In contrast, it is expected that the pressure of renewable hydrogen can be much lower and the pressurization is highly energy consuming. At present, the reaction shown above has been conducted at high H₂ pressure, and the challenge is to make the catalysts work under the conditions of low H₂ pressure.

Expected Research Achievements

● Development of "H₂ facilitators" and elucidation of their mechanism

In the reactions using H₂ as a reductant, H₂ needs to be dissociatively activated and supplied to catalytically active sites. The requirement of high H₂ pressure in the present reduction systems is due to the inhibition of H₂ activation by stronger adsorption of reactants on active sites compared to H₂. In this research, we aim to develop the materials called "H₂ facilitators" that can activate H₂, exhibit low affinity with reactant molecules, and also transport activated hydrogen efficiently to active sites. H₂ facilitators are expected to promote catalytic reactions remarkably even under low H₂ pressure. The mechanism of H₂ activation and transportation of activated hydrogen species will be elucidated. The concept of H₂ facilitation will be extended to molecular catalysis and bio-catalysis as well as solid catalysis.

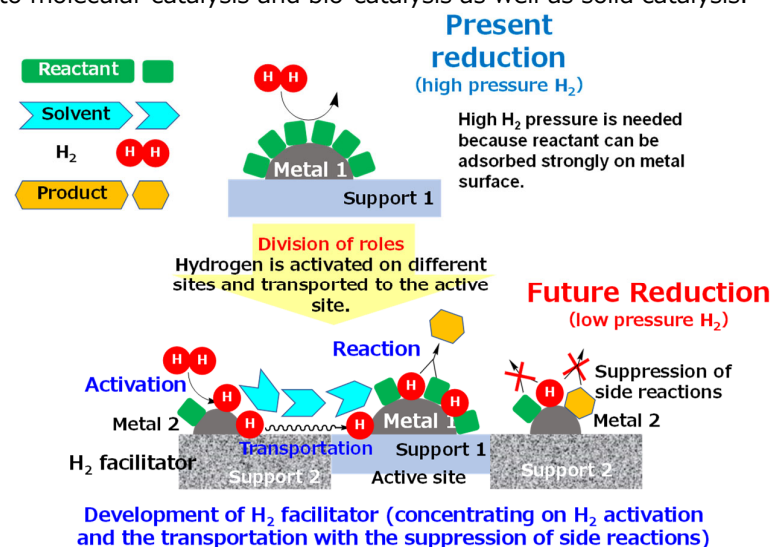


Figure 4. Problem of present reduction systems and the concept of future reduction using H₂ facilitator