【Grant-in-Aid for Scientific Research(S)】
Science and Engineering (Chemistry)

Title of Project : Development of Chemical Fixation of Ubiquitous Molecules with Bifunctional Molecular Catalysts

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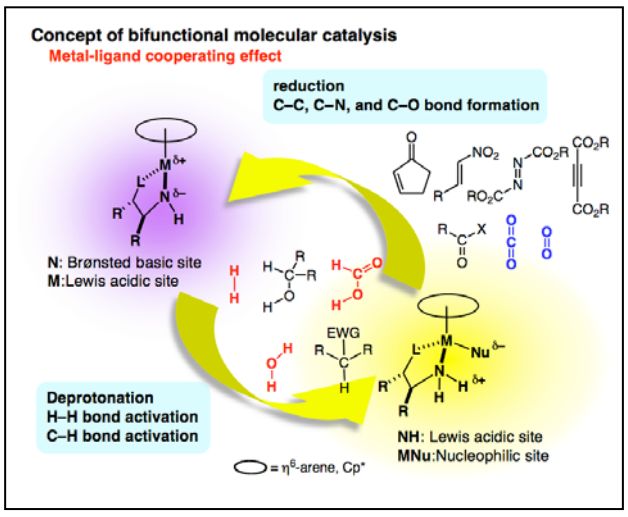
Research Area : Chemistry

Keyword : Bifunctional Molecular Catalysis, Ubiquitous Molecule, Green Chemistry

【Purpose and Background of the Research】

Catalysts are crucial not only for production of useful materials and products but also for reduction of pollution and waste of natural resources and energy. Recent advances in green and sustainable science and technology strongly demand more powerful and practical catalysts with a tunable multifunction. We have recently developed *Concerto Catalysis* based on the bifunctional molecular catalysts for highly efficient molecular transformation (Figure). This conceptually new bifunctional molecular catalysts also can activate ubiquitous molecules including H_2O, H_2, O_2, and CO_2, which are available in the Nature, and hence present an inexhaustible source of C, H, O, and N atoms. Therefore, this research focuses on exploring new methods for chemical fixation of these ubiquitous molecules by an appreciable improvement in the performance of transition metal-based bifunctional molecular catalysts.



【Research Methods】

On the basis of our accumulated knowledge in the bifunctional catalysis, we will try 1) to establish the principles of the bifunctional molecular catalysts by design and synthesis of mono- bi- and polynuclear transition metal-based complexes bearing cooperating ligands, and 2) to realize perfect chemical reactions by extension of the scope of the applicability of the bifunctional catalysis, and finally 3) to explore the chemical fixation of the ubiquitous molecules into the useful compounds and materials by development of the practical bifunctional molecular catalysts.

【Expected Research Achievements and Scientific Significance】

We believe that the emergence of powerful bifunctional molecular catalysis provides a great leap to reach more efficient, sustainable and green production processes in the field of organic synthesis. In addition, the bifunctional catalyst promoted powerful chemical fixation technology of ubiquitous molecules, H_2O, H_2, O_2, N_2, CO_2 available in huge amounts can help to replace the fossil resources. Finally, new catalytic water splitting into H_2 and O_2 that could be invented in this research project will provide an ideal method to utilize and to store solar energy.

【Publications Relevant to the Project】

・T. Ikariya, A. J. Blacker, Asymmetric transfer hydrogenation of ketones with bifunctional transition metal-based molecular catalysts. *Acc. Chem. Res.* 40, 1300–1308 (2007).
・S. Kuwata, T. Ikariya, Hydrogen- and oxygen-driven interconversion between imido-bridged dirhodium(III) and amido-bridged dirhodium (II) complexes. *J. Am. Chem. Soc.* 131, 5001–5009 (2009).
・M. Ito, T. Ikariya, Hydrogenation of *N*-acylcarbamates and -sulfonamides catalyzed by bifunctional Cp*Ru(PN) complex. *Angew. Chem. Int. Ed.* 48, 1324–1327 (2009).

【Term of Project】 FY2010-2013

【Budget Allocation】 167, 800 Thousand Yen

【 Homepage Address and Other Contact Information】

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