Institute Interest Seminar Series

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Activation of H_2 and CO by a NiIr Model Complex

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H_2 is of biological and industrial importance because it behaves as an electron donor and a fuel. However, commercially available H_2 includes a small amount of CO, which poisons the catalysts to inhibit these functions at useful rates. Oxidations of H_2 and CO in biological systems are catalyzed by [NiFe]hydrogenase ([NiFe]H_2ase) and carbon monoxide dehydrogenase (CODH), respectively. Here, we report a NiIr catalyst as models for [NiFe]H_2ase and CODH, which can oxidize either H_2 or CO, based on the pH value, in one flask (Figure 1).[1)] The NiIr catalyst can mimic the chemical function of [NiFe]H_2ase under the acidic conditions (pH 4–7) and CODH under basic condition (pH 7-10). The all Intermediates in the both catalytic cycles were isolated, whose structures were definitely determined by X-ray analysis. The NiIr catalyst can be applied to a fuel cell to promote oxidation of H_2, CO, and H_2/CO (1/1) fuel mixtures. The fuel cell's power density depends upon the pH in the fuel cell and shows a similar pH dependence in flask experiments.

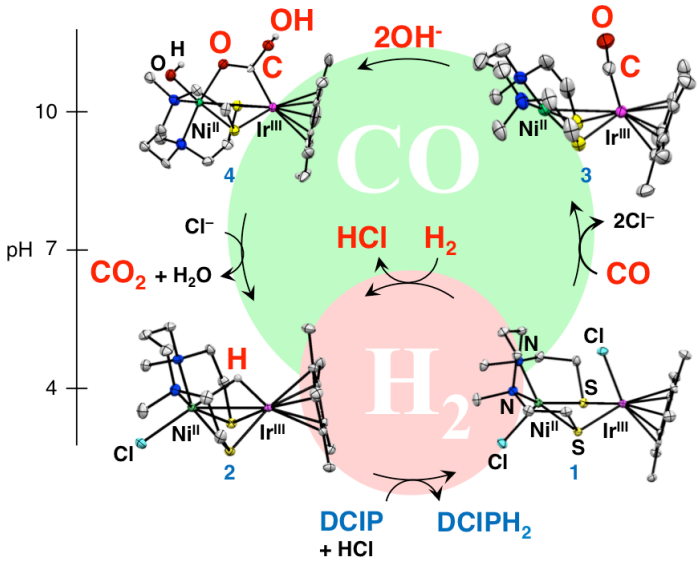

Figure 1 pH-dependent activation of H_2 and CO based on NiIr catalysts. DCIP: 2,6-dichlorobenzeneindophenol. $DCIPH_2$: two-electron reduced form of DCIP.

1) S. Ogo, Y. Mori, T. Ando, T. Matsumoto, T. Yatabe, K.-S. Yoon, H. Hayashi, M. Asano, *Angew. Chem. Int. Ed.*, **2017**, *56(33)*, 9723.