

演題：**Design of Molecular Metal
Complex and Metal Cluster
Catalyst on Supports**

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共催：触媒化学研究センター，日本化学会北海道支部

要旨：Essentially molecular rhodium and iridium catalysts were synthesized from the organometallic precursors $M(C_2H_4)_2(acac)$ (M is Rh or Ir; $acac$ is acetylacetonate) on zeolite HY and on MgO and characterized by infrared and X-ray absorption spectroscopies, atomic-resolution scanning transmission electron microscopy, and density functional theory. The supported metal complexes initially take the form of $M(C_2H_4)_2$, with two bonds between M and support oxygen atoms. These surface species have been modified to become selective for either ethylene hydrogenation or dimerization and for 1,4-butadiene hydrogenation to give either predominantly butenes or butane. The catalyst design variables are the following:

- the metal
- the ligands on the metal
- the support (which itself is a ligand)
- the metal nuclearity
- the presence of neighboring OH groups on the support
- the presence of neighboring complexes of the second metal on the support.

The chemistry occurs on surfaces; the species are essentially molecular; and the opportunities for design and control of structure, reactivity, and catalytic properties are those of molecular organometallic chemistry. Understanding requires the full complement of characterization methods mentioned above.

本講演は、大学院総合化学院『化学研究先端講義／総合化学特別研究第二』の一部として認定されています。

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