

# Lectures on October 29, Tuesday

Room Z401

09:30-10:10

## Design of Molecular Metal Complex and Metal Cluster Catalysts on Supports

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and  
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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.

10:10-10:40

**Effect of Ligands of V Complexes Encapsulated in Y-zeolite on  
Liquid-Phase Oxidation of Benzene to Phenol**

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The one-step oxidation of benzene with molecular oxygen to phenol in liquid phase was carried out by using V complexes encapsulated in Y-zeolite catalysts. The formation of V complexes in the cage of Y-zeolite prevented the elution of V species into reaction solution, and the suppression of elution sustained the activation of phenol formation. The ligand species of V complexes in encapsulated catalysts significantly affected the phenol yields. The ligand species affected on the energy gap between  $V^{3+}$  and  $V^{4+}$ , and the decrease of energy gap effectively promoted the phenol formation in this reaction.