

**“Precisely Synthesized Supported Catalysts: Understanding  
Structure and Performance at the Molecular Scale”**

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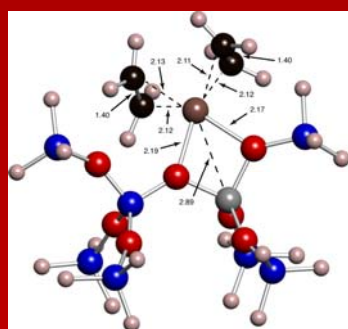
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**Abstract**

The typical industrial catalyst is a highly nonuniform set of nano-structures dispersed on a porous, nonuniform support. In contrast, some supported catalysts, such as those used for olefin polymerization, are much more nearly uniform, being molecular in character and offering the prospective advantages of molecular catalysts in solution, such as high selectivity. Our goals were to gain a deeper understanding of the class of oxide- and zeolite-supported metal catalysts with virtual molecular properties by investigating single-metal-atom complexes and clusters of only a few atoms. A key to meeting the goal of structural uniformity is precise synthesis of the supported species, by the methods of organometallic chemistry extended to surfaces. Keys to understanding of the structures and properties of these materials are characterization by complementary spectroscopic and microscopic techniques, even with the samples in reactive atmospheres. The characterization methods include vibrational, NMR, and X-ray absorption spectroscopies; scanning transmission electron microscopy; and density functional theory. The characterization results determine structures with atomic resolution, bonding of metals to supports, identification of reaction intermediates bonded to the metals, and new reaction mechanisms.

Results are presented for complexes of rhodium, iridium, and of gold on oxides and zeolites and for clusters of iridium and osmium on these supports. For example, complexes of rhodium bonded to dealuminated Y zeolite were prepared from  $\text{Rh}(\text{C}_2\text{H}_4)_2(\text{acac})$ , giving supported  $\text{Rh}(\text{C}_2\text{H}_4)_2$  complexes with each Ir atom bonded to two O atoms of the zeolite, as shown below:



Other examples include 3-atom clusters of osmium and 6-atom clusters of iridium. Details of reaction mechanisms are presented for supported rhodium and iridium complexes and clusters catalyzing reactions of olefins and hydrogen. These supported molecular catalysts are an emerging class of materials expected to offer new reactivities and catalytic properties. Some of the lessons emerging from understanding of their structure and bonding pertain to supported metal catalysts generally.

**Biographical Sketch**

Dr. Gates joined the University of California, Davis in 1992. His research interests are: catalysis, nanomaterials, surface chemistry, organometallic surface chemistry, new catalytic materials, reaction kinetics, and chemical reaction engineering. Applications to petroleum refining, petrochemical processing, and coal conversion. Catalytic hydroprocessing, catalysis by synthetic polymers, strong acids, zeolites, and supported transition metal complexes and nanoclusters.

In 2009, Gates was awarded the North American Catalysis Society's 2009 Robert Burwell Lectureship in Catalysis, which recognizes four decades of significant contributions in three major areas of catalysis research. Gates also was commended for having mentored more than 130 students, postdocs and visiting scientists, and for having educated two generations of catalytic scientists and industrial practitioners.