

# CHEMICAL ENGINEERING

## SEMINAR SERIES



**BRUCE GATES**

**10/10/16**

Professor of Chemical Engineering  
University of California - Davis

## Molecular Metal Catalysts on Supports: Organometallic Chemistry Meets Surface Science

**ABSTRACT:** Industrial catalysts range from the simple—molecules in solution—to the complex—surfaces of robust solids, and these are represented respectively by the fields of organometallic chemistry and surface science. These fields are now rapidly merging, benefiting from synthetic chemistry showing the way to essentially molecular metal-containing species anchored on solid supports. The best understood of these catalysts are highly uniform, being isolated on crystalline supports such as zeolites and metal organic frameworks. Less uniform supports such as crystalline MgO are helping to move this field a step closer toward the complexity of technological catalysts incorporating metal oxide supports. The catalyst syntheses involve reactions of organometallic compounds (e.g.,  $\text{Ir}(\text{C}_2\text{H}_4)_2(\text{acetylacetonate})$ ) with OH groups on support surfaces—to give structures such as  $\text{Ir}(\text{C}_2\text{H}_4)_2$ , with the Ir atom bonded to two support oxygen atoms. Spectra, atomic-resolution electron microscopy images, and calculations at the level of density functional theory characterize the surface structures and demonstrate their high degrees of uniformity. Catalyst performance data representing families of isostructural catalyst precursors, such as  $\text{M}(\text{C}_2\text{H}_4)_2$ ,  $\text{M}(\text{CO})(\text{C}_2\text{H}_4)$ , and  $\text{M}(\text{CO})_2$  ( $\text{M} = \text{Rh}, \text{Ir}$ ), show how the metals and ligands affect catalytic properties—just as in molecular homogeneous catalysis. New catalysts provide potentially valuable properties, such as high selectivity for hydrogenation of 1,4-butadiene to give butenes catalyzed by selectively poisoned dirhodium species on MgO. The new results are helping to unravel the effects of the design variables of site-isolated catalysts: the metal, the number of metal atoms in a catalytic site, the support, and other groups (ligands) bonded to the metal—thereby laying a foundation for a role of theory in catalyst design.

**RECEPTION 3:30 • LECTURE 4:00 - 5:00**  
**PHYSICS ASTRONOMY BLDG. (PAA) A110**



**CHEMICAL ENGINEERING**

UNIVERSITY of WASHINGTON

*Knowledge and solutions for a changing world*

**BIOGRAPHY:** Bruce C. Gates, a PhD alumnus of the University of Washington, teaches in the Department of Chemical Engineering at the University of California, Davis, and formerly he taught at the University of Delaware and worked at Chevron. His research group is active in catalysis, with a focus on supported metal complex and metal cluster catalysts that are essentially molecular and lend themselves to design and in-depth characterization by spectroscopy and atomic-resolution microscopy. His group also works on catalysis of biomass conversion, with a focus on hydroprocessing. Gates wrote the textbook *Catalytic Chemistry* and coauthored the textbook *Chemistry of Catalytic Processes*. Until recently, he edited *Advances in Catalysis*. He serves on the U.S. Department of Energy's Basic Energy Sciences Advisory Committee and the North American Catalysis Society's Board of Directors.