SEMINAR SERIES

International Institute for Carbon-Neutral Energy Research
Kyushu University

Title Hydrogen activation in molecular complexes: Chemical approaches to catalysis and energy storage

Speaker Dr. Tom Autrey
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Date & Time Friday, April 27, 2012 4:00p.m.

Place INAMORI Hall, Ito campus, Kyushu University

Abstract

Novel approaches for activating hydrogen are needed to increase efficiency and decrease costs in energy-intensive industrial processes. Amine boranes have the potential to provide unique solutions to two seemingly different applications: (i) catalytic hydrogenation, critical to many industrial processes, ranging from upgrading crude oil to ammonia synthesis, and (ii) hydrogen storage, a potentially critical solution to storing energy from intermittent renewable sources such as wind and solar.

In this presentation we discuss the relationship between hydrogen storage and catalysis. Our work starts with the pedagogical example of ammonia borane and ammonium borohydride in hydrogen storage and extends to more complex amine borane structures that provide the ability to tune thermodynamics. We describe a combination of experimental and computational approaches to gain insight into structure and reactivity of non-metal molecular complexes composed of Lewis acid Lewis base functionality to understand the mechanism of heterolytic activation of molecular hydrogen.

About the Speaker

Tom Autrey is a Staff Scientist in the Fundamental and Computational Science Directorate at the Pacific Northwest National Laboratory. Dr. Autrey's current research interests are focused on small molecule activation for catalysis and approaches to energy storage for fuel cell power applications. He is the Principle Investigator on the US DOE Office of Science Catalysis Science Program, Activation of Small Molecules with Bi-functional Ambiphilic Catalyst Complexes, and a Co-Principle Investigator on the US DOE Office of Energy Efficiency and Renewable Energy's Hydrogen Storage Novel Carbon-Boron-Nitrogen Containing H2 Storage Materials. Dr Autrey serves on the Lujan Center Neutron review committee at LANSCE, as a panel expert on the International Energy Agency task on Hydrogen Storage and as a member of the US DOE Technical Team advising on Hydrogen Storage for vehicle applications. In 2006 he was awarded the DOE - Energy Efficiency and Renewable Energy Award for "Research in Hydrogen Storage". Dr. Autrey has several national and international collaborations designed to combine experimental and computational approaches to study complex phenomena in chemical materials.

Host: Professor Etsuo AKIBA

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