Partner Institutions

IACT partners include Argonne National Laboratory, Brookhaven National Laboratory, Northwestern University, Purdue University, and the University of Wisconsin-Madison.

Facilities

IACT employs the following state-of-the-art research facilities across the United States.

Argonne National Laboratory

- Advanced Photon Source
- Center for Nanoscale Materials
- Advanced Leadership Computing Facility
- Electron Microscopy Center

Brookhaven National Laboratory

- Center for Functional Nanomaterials

Northwestern University

- Northwestern University Atomic and Nanoscale Characterization Experimental Center (NUANCE)

Purdue University

- Birck Nanotechnology Center

Strategic Alliances with Other Energy Frontier Research Centers

In addition to its partner institutions, IACT also shares collaborative relationships with the following Energy Frontier Research Centers (EFRCs).

EFRC Name	Collaborative Focus
Center for Direct Catalytic Conversion of Biomass to Biofuels (C3Bio) Purdue University	Understanding the fundamental building blocks of biomolecules and how the nature of these materials effects their ultimate catalytic conversions
Catalysis Center for Energy Innovation (CCEI) University of Delaware	Synthesis of site-specific catalysis and development of in situ cells for synchrotron studies
Center for Atomic-level Catalyst Design (CALC-D) Louisiana State University	Developing and implementing new computational tools for simulating catalyst surfaces and reactivity
Fluid Interface Reactions, Structures and Transport (FIRST) Oak Ridge National Laboratory	Understanding the interactions of solid-liquid interfaces important to the liquid phase conversion of biomass

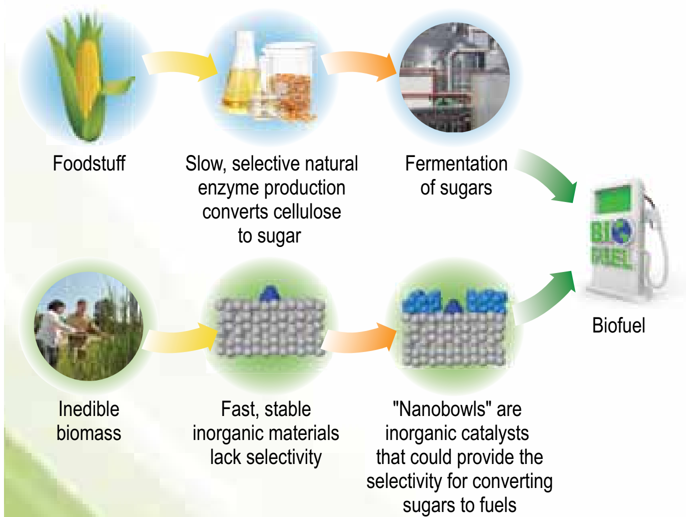
Institute for Atom-efficient Chemical Transformations
Argonne National Laboratory
9700 S. Cass Avenue
Argonne, IL 60439

www.iact.anl.gov

Institute for Atom-efficient Chemical Transformations (IACT)

Dedicated to advancing the science of catalysis for efficient conversion of bioresources, improving the efficiency for conversion of biomass to fuels, and promoting the selective removal of oxygen

Current Process Uses Organic Enzymes to Produce Biofuels



IACT Proposes Synthetic, Inorganic Catalysts to Produce Biofuels

U.S. DEPARTMENT OF ENERGY

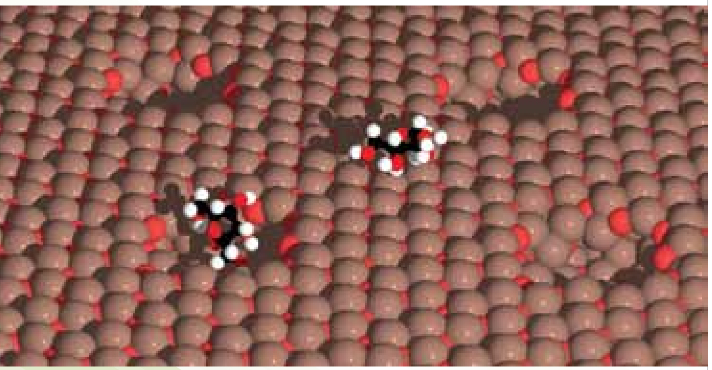
IACT is an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

Leveraging a Multidisciplinary Approach to Catalysis Science

IACT researchers work to achieve control and efficiency of chemical conversions comparable to those in nature, which requires new materials. IACT's major emphasis is synthesis of new, complex, multisite, multifunctional catalytic materials that offer new models for catalysis. Advanced computation and modeling tools help to interpret, understand, and optimize experimental results.

IACT research focuses on four primary tasks:

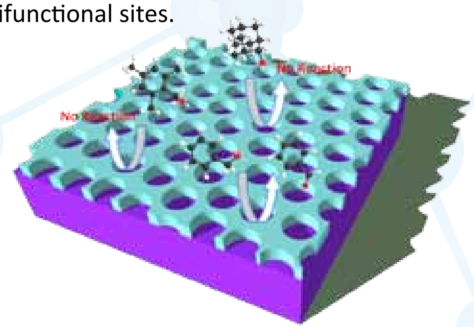
- Synthesis
- *In situ* Characterization
- Computational Modeling
- Chemical and Catalytic Reaction Science



Fructose molecules adsorbed on a zirconium oxide surface (right) and in a zirconium oxide nanobowl (left). The brown atoms are surface oxygen and the coral atoms are zirconium. Carbon, oxygen, and hydrogen atoms of fructose molecules are shown in black, red, and white, respectively.

Synthesis

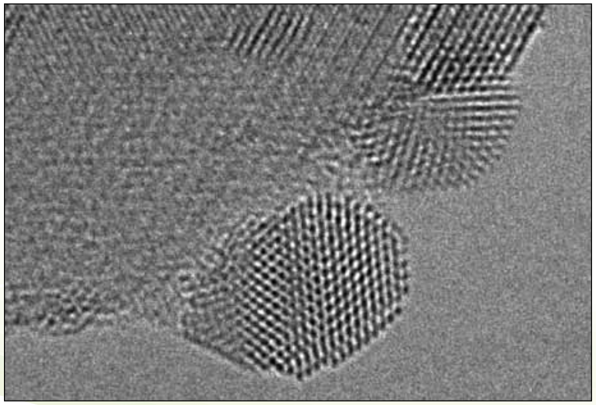
In the Synthesis task, researchers focus on developing new, complex, multisite, multifunctional catalytic materials, including isolated monofunctional sites, proximate multifunctional sites, and synergistic multifunctional sites.



Preparation of single-site "nanobowl" (inorganic catalyst) that can be used to study catalytic behavior.

In situ Characterization

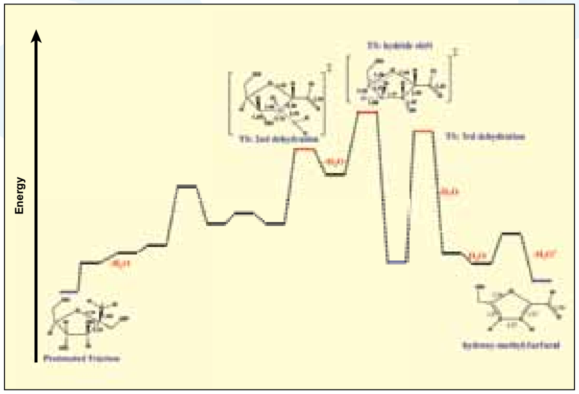
Scientists use *in situ* characterization of catalyst structure, composition, and function to reveal the "real-world" atomic scale processes controlling catalysis, and then apply a variety of spectroscopic tools to provide fundamental understanding.



In situ imaging and spectroscopy tools facilitate characterization of catalyst structure.

Computational Modeling

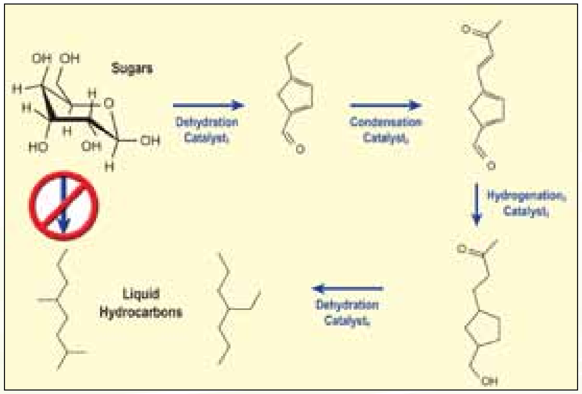
Modeling tools assist in interpreting, understanding, and optimizing experimental results, by facilitating development of theoretical insights at the atomic level, providing guidance in the discovery of new catalytic materials.



Exploration of reaction pathways supports development of new theoretical insights at the atomistic level.

Chemical and Catalytic Reaction Science

In examining the performance of new materials for catalyzing reactions of interest, IACT researchers focus on carbohydrates, lignin and lignite, and cellulose.



Many individual catalytic steps will be required to convert cellulosic sugars into fuels. IACT is examining these key reactions to understand the fundamental chemistry and to provide improved catalytic performance.