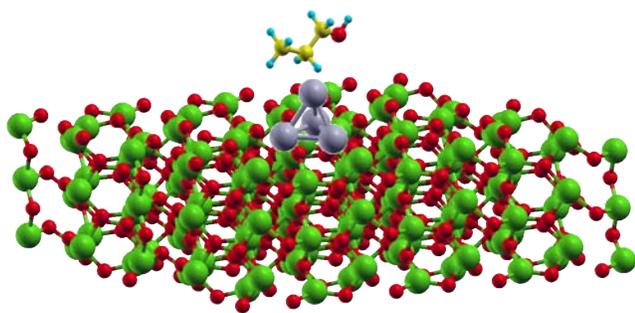


Institute for Atom-Efficient Chemical Transformations (IACT)

The Institute for Atom-Efficient Chemical Transformations (IACT) focuses on advancing the science of catalysis for the efficient conversion of energy resources into usable forms.

IACT is a partnership among world-class scientists at Argonne National Laboratory, Northwestern University, University of Wisconsin-Madison, and Purdue University. Using a multidisciplinary approach involving integrated catalyst synthesis, advanced characterization, catalytic experimentation, and computation, IACT will address key chemistries associated with clean, efficient utilization of the two main chemical energy resources in the United States, namely coal and biomass. We have identified the efficient removal of oxygen from biomass and coal and the hydrogenation of these systems as key chemistries and unifying themes for IACT.



Nature's catalysts — enzymes — show how amazingly efficient chemical transformations can be. IACT researchers believe that the control, efficiency, and selectivity of chemical conversions comparable to those achieved by Nature are within the reach of synthetic catalysts. This achievement will require new catalytic materials, and a major IACT emphasis is the design and synthesis of new, complex, multisite, multifunctional catalytic materials offering new paradigms for catalysis.

To understand these new catalytic materials, an integrated characterization effort is required. In some cases, important questions about catalyst structure, composition, and function can be answered only through advances in measurement science, and this is an important aspect of IACT research. Closely coupled interpretation, understanding, and prediction of experimental results by computation is also critical to advancing catalysis science and is a major IACT activity. Finally, the ultimate validation of our synthesized, characterized, and computationally modeled catalysts will come from characterizing their catalytic performance, as will feedback for further catalyst design.

Thus, IACT may be viewed as consisting of four distinct but intimately interlinked task areas: synthesis, characterization, computation, and chemical and catalytic reaction science.

The leaders of each subtask area are experts in the disciplines constituting its activities. For example, in the synthesis task area, both molecular and materials synthesis are required, and each leader is expert in one of these areas. The integration and interdependence of subtasks follows naturally from the needs that each has for the others to answer basic scientific questions. This integration and interdependence is ensured by an effective management structure whose membership cuts across subtask expertise, and through regular communication via meetings, seminars, and collaborations.



Catalyst Synthesis

IACT researchers will concentrate on three primary classes of materials:

- **Isolated Mono-Functional Sites**
Conventional picture of heterogeneous catalysis, such as oxide-supported metal particles or an acid/redox site on a bulk oxide.
- **Proximate Multi-Functional Sites**
Catalysts in which multiple functions, such as metal and acid, are positioned in three dimensions with separations on the nanoscale or less.
- **Synergistic Multi-Functional Sites**
Catalysts with two or more surface functionalities are in such close proximity that they act simultaneously on a single functional group in the reactant molecule.

Synthesis will seek to control not only the chemistry of the active site but also the geometrical and chemical nature of the support that anchors these catalytic moieties. IACT scientists believe that control of both the active site and the support are necessary to provide catalysts that mimic natural enzymes.

In Situ Characterization

IACT researchers will investigate synthesized materials under “real world” conditions, studying the atomic-scale processes that control catalysis. This task will provide insights to develop physically based predictive models of the property of materials synthesized. In situ characterization will employ a variety of spectroscopic tools to provide fundamental understanding regarding why the superior catalysts perform so well and why inferior materials fail completely or deactivate too quickly.

Computational Modeling

Computational modeling will provide theoretical insights at the atomistic level regarding the catalytic properties of new materials and experimental observations. Modeling will also provide guidance in the discovery of new catalytic materials.

Catalytic and Chemical Reaction Science

Catalytic and chemical reaction science will provide data on how the synthesized materials control the fundamental chemistry of oxygen removal from carbohydrates, lignin, and lignite. Since the reactants in transformations are multi-functional molecules, selective transformation of one function but not another will be critical to developing and exploring efficient chemical conversion processes.

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