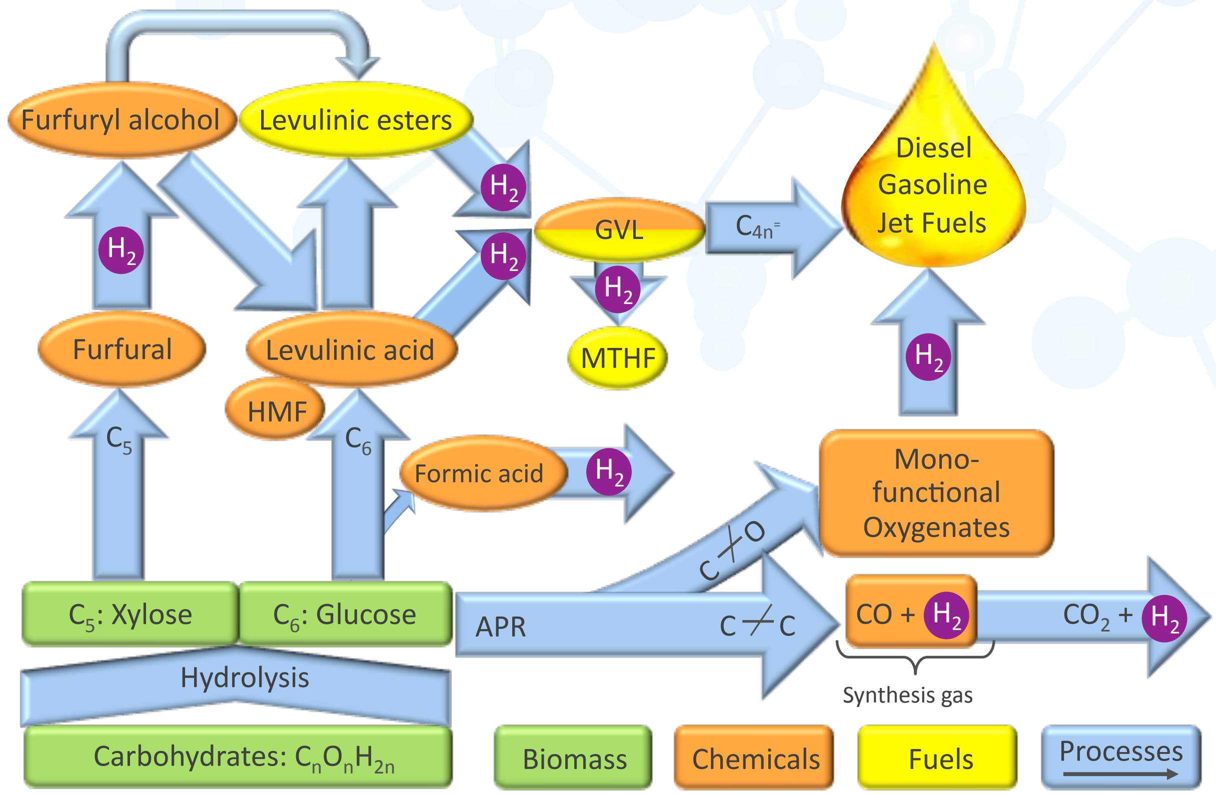
## Biomass Roadmap




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

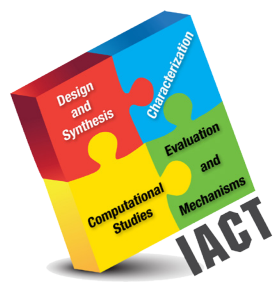
Argonne NATIONAL LABORATORY

BROOKHAVEN NATIONAL LABORATORY

NORTHWESTERN UNIVERSITY

PURDUE UNIVERSITY

WISCONSIN UNIVERSITY OF WISCONSIN–MADISON





**Institute for Atom-efficient Chemical Transformations**

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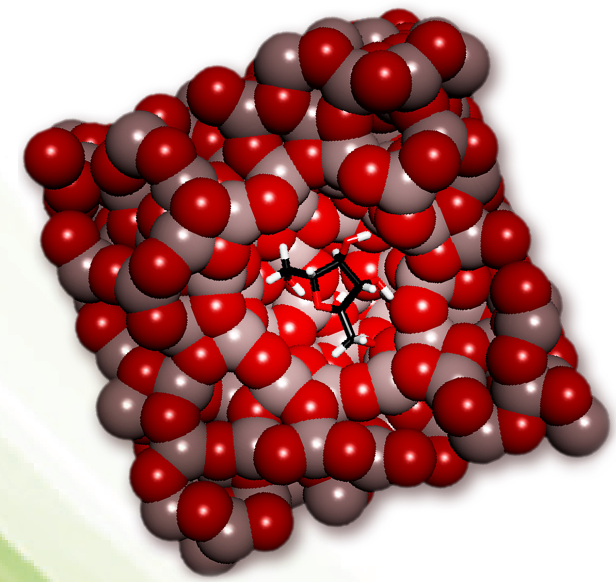
# Institute for Atom-efficient Chemical Transformations (IACT)

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



IACT Proposes Synthetic, Inorganic Catalysts to Produce Biofuels


U.S. DEPARTMENT OF ENERGY

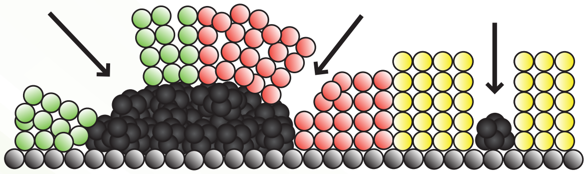
IACT is an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

# Leveraging a Multidisciplinary Approach to Catalysis Science

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

IACT research encompasses four primary tasks:

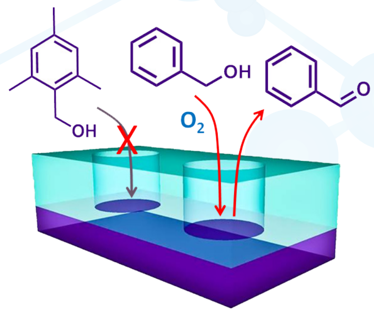
- Synthesis
- *In situ* Characterization
- Computational Modeling
- Chemical and Catalytic Reaction Science



*Atomic Layer Deposition over the top of metals (left, red and green areas) can modify catalyst selectivity by blocking specific sites. Metal nanoparticles embedded in "nanobowls" (right, yellow area) maintain activity and exhibit shape-selective catalysis.*

# Synthesis

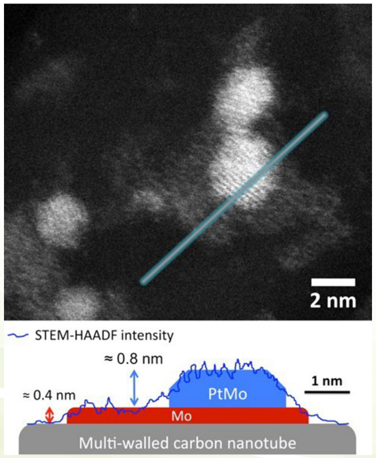
In the Synthesis task, researchers focus on developing new, complex, multisite, multifunctional catalytic materials, including isolated monofunctional sites, proximate multifunctional sites, and synergistic multifunctional sites.




*Nanobowls can be used to study size-selective catalytic behavior.*

# *In situ* Characterization

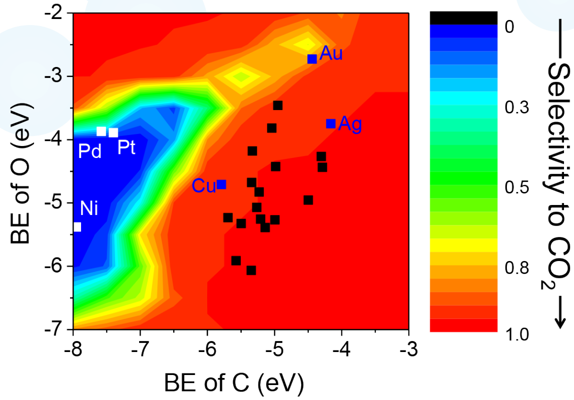
IACT scientists use *in situ* characterization of catalyst structure, composition, and function to reveal the "real-world" atomic scale processes controlling catalysis, and then apply a variety of spectroscopic tools to provide fundamental understanding.




*High-Angle Dark Annular Field image of a PtMo alloy catalyst (top). Model based on high-resolution spectroscopic imaging resolves the catalyst's structure (bottom).*

# Computational Modeling

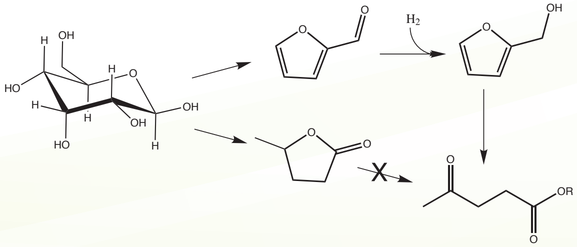
Modeling tools assist in interpreting, understanding, and optimizing experimental results, by facilitating development of theoretical insights at the atomic level, providing guidance in the discovery of new catalytic materials.




*Selectivity of formic acid decomposition to $CO_2$ as a function of the binding energies of O and C to metal surfaces. Image shows volcano plots derived from microkinetic modeling.*

# Chemical and Catalytic Reaction Science

In examining the performance of new materials for catalyzing reactions of interest, IACT researchers focus on the reaction mechanisms involving 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.*