Institute for Atom-efficient Chemical Transformations (IACT)
EFRC Director: Christopher L. Marshall
Lead Institution: Argonne National Laboratory

Mission Statement: *To address key catalytic conversions that could improve the efficiency of producing fuels from biomass. IACT is focusing on advancing the science of catalysis for the efficient conversion of energy resources into usable forms. IACT's goal is to find ways to achieve control and efficiency of chemical conversions comparable to those in nature.*

Vision: The focus of IACT is to advance the science of catalysis for the efficient conversion of renewable energy resources into usable forms. IACT is a partnership among world-class scientists at Argonne National Laboratory, Northwestern University, University of Wisconsin-Madison, Purdue University, and Brookhaven National Laboratory. Using a multidisciplinary approach involving new catalyst synthesis, advanced characterization, catalytic experimentation, and computation, IACT addresses three catalytic conversions that are key to improving the efficiency for conversion of biomass to fuels: 1) selective removal of oxygen by dehydration, 2) selective hydrogenation of oxygen containing functional groups, and 3) C-C bond formation. The grand vision for IACT is to create a knowledge base for these key transformations that guides efficient deconstruction of biomass and enables highly selective conversion of the resulting oxygenated molecules to fuel components with minimum loss of the precious carbon that was fixed by photosynthesis to create the biomass. Thus, precise control of reaction pathways is our main mission.

To achieve this mission, IACT consists of four distinct, but intimately interlinked subtasks: synthesis, characterization, computation, and chemical and catalytic reaction science (see diagram on next page). The integration and interdependence of these subtasks follow naturally from the needs that each has for the others to answer basic scientific questions. This integration and interdependence are ensured by (i) an effective management structure, whose membership cuts across subtask expertise, and (ii) regular communication among participants via meetings, seminars, and collaborations.

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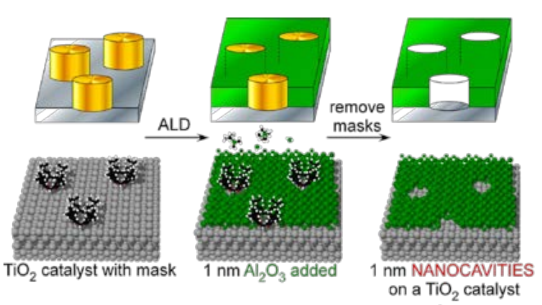
<tr><th>Research Goals</th><th>Key Progress Milestones</th></tr>
<tr><td>Synthesis of nanobowls for the controlled catalysis and protection of small metal particles.


Schematic for templated synthesis of nanobowls in an Al_2O_3 layer on a TiO_2 particle.</td>
<td>• Established the shape- and size-selectivity of nanobowl catalysts prepared by templated ALD for the photocatalytic oxidation of alcohols.
• Demonstrated enhanced thermal stability and selectivity of ALD over-coated noble metal nanoparticle catalysts.</td></tr>
<tr><td>Improved catalyst activity and selectivity for the reforming of small alcohols.</td>
<td>• Developed a series of highly active and stable bimetallic catalyst has been discovered which produces hydrogen from biomass under aqueous reaction conditions.</td></tr>
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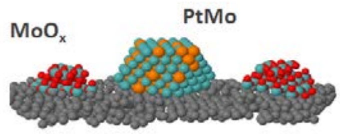
<td>

Alloying Pt with less noble metals (e.g. Mo or Co) improves activity and selectivity for aqueous phase reforming reactions.</td>
<td>• Synthesized a highly active and selective new bimetallic catalyst has been discovered, which hydrogenates oxygen-rich biomolecules to gasoline-compatible fuels under aqueous reaction conditions.</td>
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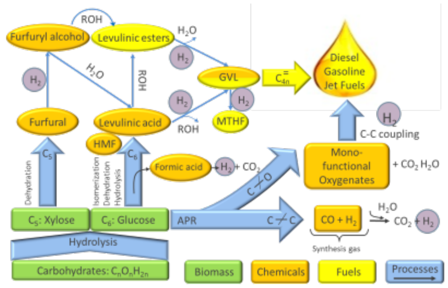
<td>Improved fundamental understanding in the catalytic conversion of furfural to levulinic acid.


Overall scheme of reactions being explored within IACT for the conversion of cellulosic biomass to transportation fuels.</td>
<td>• Identified that one of the major reaction pathways for conversion in liquid water of furfuryl alcohol to levulinic acid takes place via a geminal diol species formed by the addition of two water molecules.
• Identified multiple reaction pathways for conversion of furfuryl alcohol in ethanol solvent to ethyl levulinate, one of which leads to the co-production of diethylether.</td>
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<td>Selective conversion of glucose and fructose to chemical intermediates.</td>
<td>• Concluded a theoretical and experimental study of the pathways and intermediates for the conversion of fructose to hydroxymethylfurfural (HMF) in dimethyl sulfoxide. HMF is a desirable compound for further processing into chemical feedstocks.
• Showed that high level calculations can provide detailed data on the energetics and pathways for a variety of relevant reactions including lactic acid hydrogenation to propylene glycol and propanoic acid on Pt(111), and the mechanism for furfural hydrogenation and decarbonylation on transition metal surfaces.</td>
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