CATALYSIS R&D CAPABILITIES AT NATIONAL LABORATORIES

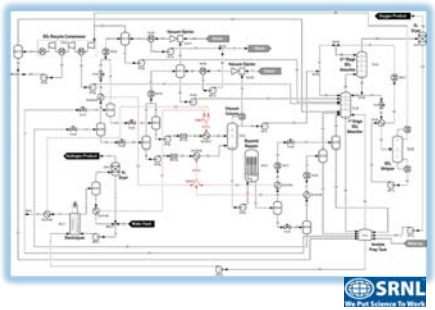
Process concept, catalyst design, synthesis, characterization and scale-up

The National Laboratories have outstanding catalysis capabilities and expertise to address national needs in catalyzed chemical transformations and energy conversion.

- Capabilities from concept and design to characterization to scale-up
- Available for industrial collaboration and through access at user facilities
- Currently engaged in industry collaboration (see Catalysis Solutions poster)

Process Concept and Design

- National Laboratories have deep expertise in design of chemical and catalytic processes for synthesis and alternative energy conversion pathways.
- Experienced in industrial collaboration.



Hybrid sulfur-cycle flowsheet for hydrogen production. Example of advanced (steady-state and dynamic) equipment modeling and flowsheet design. Operations are modeled using accurate properties in continuous, semi-batch, batch, and discrete event processes.

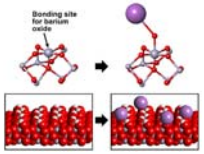
Computational Catalyst Function/Design

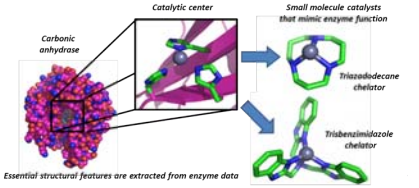
National laboratories model catalyst function and mechanism at the molecular level.

- Homogeneous and heterogeneous catalysis.
- Advanced computational facilities – access and expertise
- Design of new catalysts from first principles, or from inspiration of enzyme-based efficient biological catalysis.

Computational methods contributed to understanding oxide supported lean NOx trap (LNT) catalysts.

Pacific Northwest NATIONAL LABORATORY





Lawrence Livermore National Laboratory

Improved catalysts for CO_2 reduction catalysis have been inspired by understanding enzyme function.

Scale-Up and Process Integration

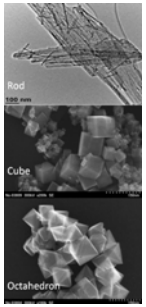
National Laboratories have extensive experience in scale-up and process integration of catalysis-based chemical transformations

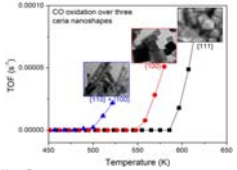
Chemical process development involving engineers, chemists, materials scientists, and computational physicists to build models from lab scale data for process scale-up. Capability for harsh environments (pressure, temperature, acid, base)

Advanced Catalyst Synthesis

Unique resources for catalyst synthesis

- Highly controlled nanostructured and nanoporous solids
- Oxides, polymers, organometallics, metals and metal alloys
- High throughput synthesis and testing.



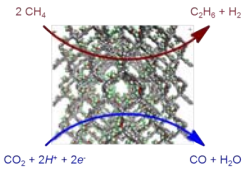


OAK RIDGE National Laboratory

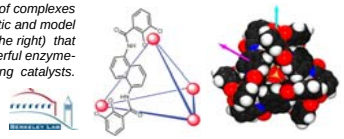
Specially synthesized CeO_2 nanoparticles with uniform crystallographic terminations provide a tool to probe relation between surface structure and surface reactivity.

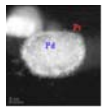
Permanently porous organic polymers (POPs) incorporate highly selective organometallic active sites in a spatially determined environment to control reaction pathway.

Argonne NATIONAL LABORATORY

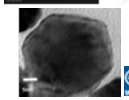


A new class of complexes (schematic and model structures at the right) that function as powerful enzyme-mimicking catalysts.





BROOKHAVEN NATIONAL LABORATORY



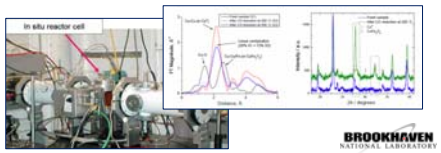
SRNL We Put Science To Work

Core-shell catalysts and electrocatalysts have unique properties while lowering noble metal cost. For example, high oxygen reduction reaction activity and durability with ultra-low Pt content using a monolayer Pt shell on an optimized core.

In Situ (In Operando) Characterization

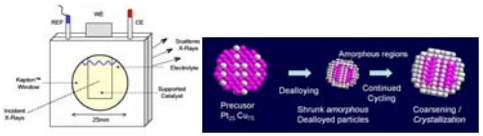
World class instruments for the characterization of catalyst structure, chemical state and function.

- Characterization under the conditions of operation.
- Captures catalyst state at temperature and pressure.
- In contact with reactive gasses or at the liquid-solid interface.



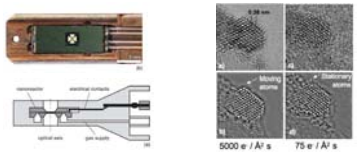
BROOKHAVEN NATIONAL LABORATORY

Combined XAFS/XRD characterize changes in catalyst under reaction conditions - Synchrotron Catalysis Consortium

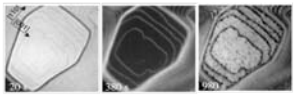


SLAC

In Situ x-ray studies of electrocatalysts during operation show changes important to durability.



Atomic resolution imaging at temperature and under gases by environmental transmission electron microscopy.



Sandia National Laboratories

Electrochemical LEEM/PEEM provides 10 nm resolution and chemical sensitivity for real-time imaging of dynamic processes.

U.S. DEPARTMENT OF ENERGY Office of Science

Lawrence Berkeley National Laboratory