NREL
NATIONAL RENEWABLE ENERGY LABORATORY

NATIONAL
BIOENERGY CENTER

NREL'S CAPABILITIES IN **CATALYST DEVELOPMENT AND CHARACTERIZATION**

CORE CAPABILITIES AND APPLICATIONS

NREL works to understand structure-performance relationships for advanced catalytic materials to enable improved carbon yield and reduced costs for the conversion of renewable feedstocks. Focus areas include:

- Innovative synthetic routes to catalysts with controlled structures and functional surface chemistries
- Detailed cost estimation for bulk-scale manufacturing of pre-commercial catalysts
- Collaboration with industrial catalyst manufacturers to guide development of scalable catalyst formulations
- Catalytic and electrocatalytic upgrading of real biomass and waste resources to fuels and chemicals
- *In situ* and *operando* characterization of catalysts and products during evaluation with real feedstocks (e.g., whole biomass vapors)
- Understanding catalyst deactivation and developing effective regeneration protocols.

Top Photo: NREL researchers discuss catalyst deactivation in the Biomass Surface Characterization Laboratory. *Photo by Dennis Schroeder, NREL 38812*

Bottom Photo: CatCost™ developers from NREL talk about the catalyst cost estimating tool's data visualizations. *Photo by Dennis Schroeder, NREL 56072*

CATALYST DESIGN AND SYNTHESIS

NREL researchers accelerate catalyst development by pioneering innovative synthetic strategies to access targeted catalyst structures. For example, solution-synthesis approaches have enabled control over catalyst composition, morphology, and surface functionalization, promoting highly selective chemical transformations. Guided by in-house computational modeling and characterization, critical catalyst features can be tailored to meet performance and cost targets.

CATALYST PRODUCTION COST ESTIMATION

The CatCost™ tool is a user-friendly, publicly available spreadsheet and web-based estimator that enables researchers to determine the cost to manufacture pre-commercial catalysts at any stage during their development. It provides quantitative cost information and powerful visualizations to help inform catalysis research and development.

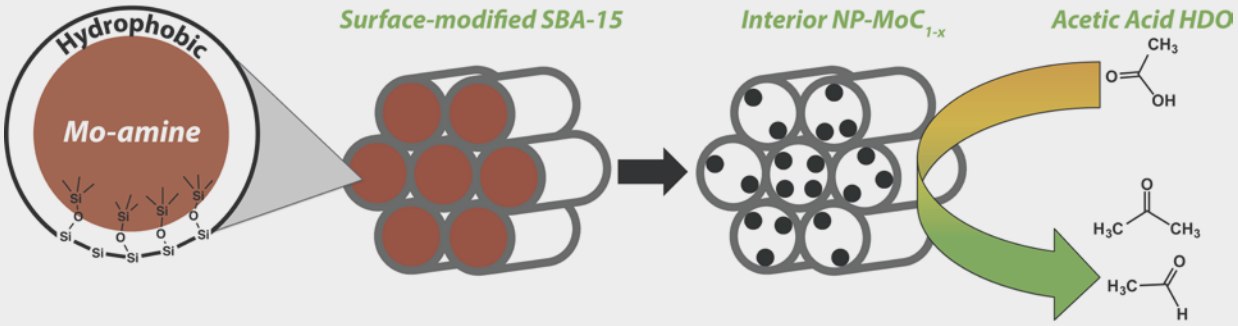
CATALYST CHARACTERIZATION AND PRODUCT ANALYSIS

NREL's comprehensive catalyst characterization and product analysis capabilities enable detailed understanding of catalyst composition and its impact on performance. Many of these capabilities have been designed specifically for in situ and *operando* characterization of the working catalyst, such as in situ titrations coupled with molecular beam mass spectrometry product analysis.

CONVERSION OF RENEWABLE FEEDSTOCKS TO FUELS AND CHEMICALS

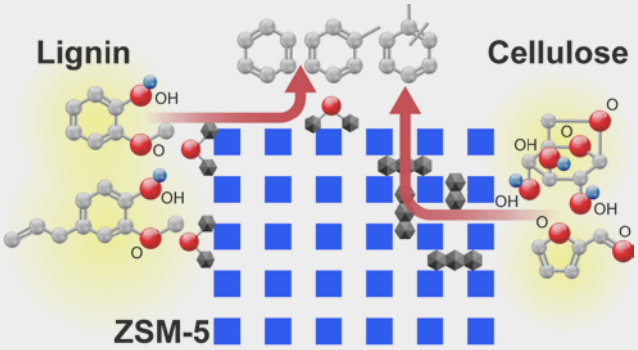
Evaluation and characterization of catalysts in integrated reactor systems with real biomass and waste streams offers direct feedback on how targeted catalyst modifications impact critical properties such as deactivation, leading to new catalysts with enhanced lifetime.

RECENT SUCCESSES



NREL researchers developed a new synthetic method for making nanoscale metal carbides that enables control of deoxygenation and hydrogenation on carbide catalysts through spatially confined nanoparticle growth.

Recent work at NREL identified the different mechanisms by which the cellulose and lignin components of biomass form coke and cause deactivation over a zeolite catalyst.



Highlighted Publications

M. Jarvis, et al. "Catalytic Upgrading of Biomass Pyrolysis Oxygenates using a Davison Circulating Riser Reactor." *Energy and Fuels*. DOI: 10.1021/acs.energyfuels.7b02337.

S.E. Habas, et al. "High-Throughput Continuous Flow Synthesis of Nickel Nanoparticles for the Catalytic Hydrodeoxygenation of Guaiacol." *ACS Sus. Chem. Eng*. DOI: 10.1021/acssuschemeng.6b02009.

C.A. Farberow, et al. "Exploring Low-Temperature Dehydrogenation at Ionic Cu Sites in Beta Zeolite to Enable Alkane Recycle in Dimethyl Ether Homologation." *ACS Catal*. DOI: 10.1021/acscatal.6b03582.

S.E. Habas, et al. "A Facile Single-Source Molecular Precursor Route to Metal Phosphide Nanoparticles and Their Evaluation as Hydrodeoxygenation Catalysts." *Chem. Mater*. DOI: 10.1021/acs.chemmater.5b02140.

Find Out More

For more information and collaboration opportunities, contact:

Kim Magrini, kim.magrini@nrel.gov
Susan Habas, susan.habas@nrel.gov
Frederick Baddour, frederick.baddour@nrel.gov

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National Renewable Energy Laboratory
15013 Denver West Parkway
Golden, CO 80401

303-275-3000 • www.nrel.gov

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