ChemCatBio
Chemical Catalysis for Bioenergy

BETO 2021 Peer Review:

# Overview of the Chemical Catalysis for Bioenergy Consortium

Josh Schadle

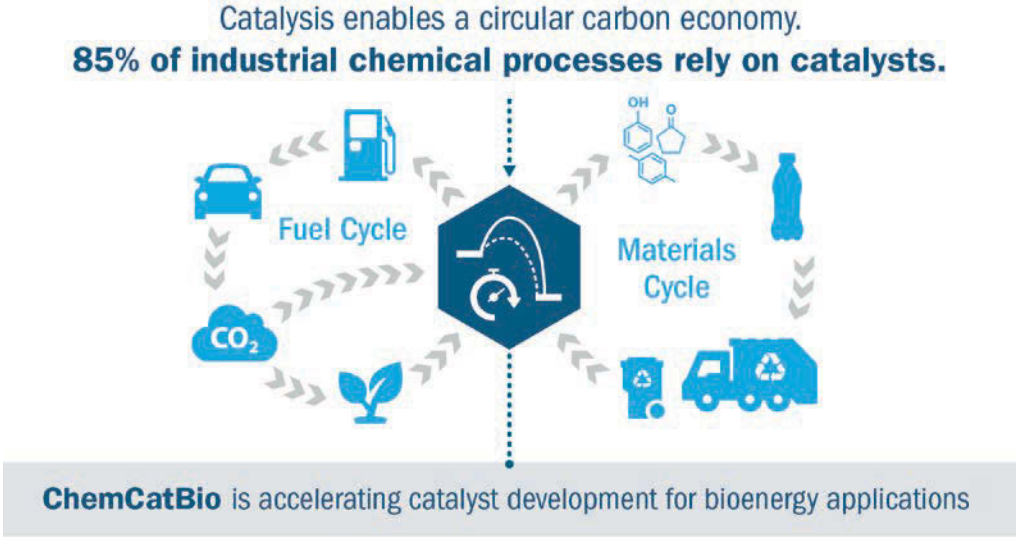
Catalytic Upgrading
March 9th, 2021

U.S. DEPARTMENT OF ENERGY | Office of ENERGY EFFICIENCY & RENEWABLE ENERGY
BIOENERGY TECHNOLOGIES OFFICE

# **Project Overview:** ChemCatBio Mission

**Mission:** Accelerate the catalyst and process development cycle for bioenergy applications

**Vision:** A rapid transition to a circular carbon economy

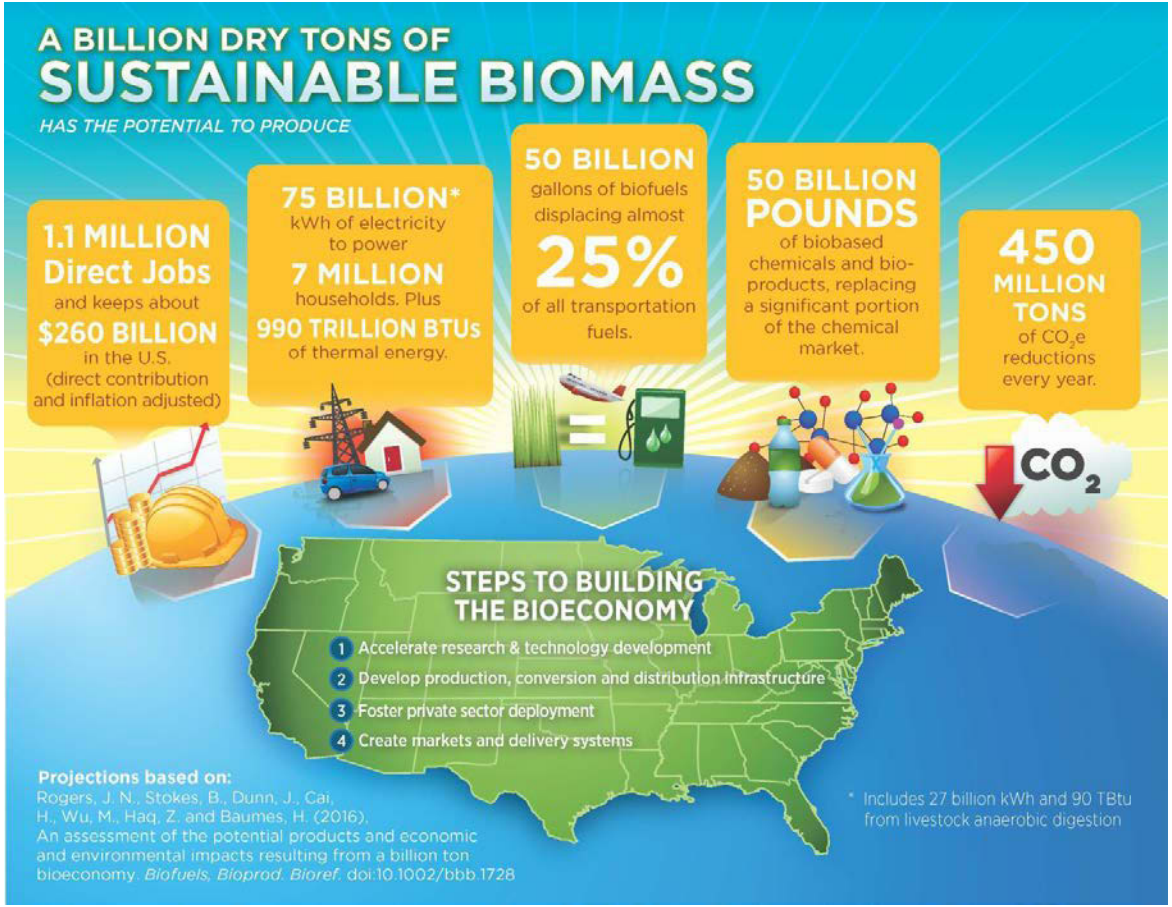



## Potential Future Impact of Catalysis

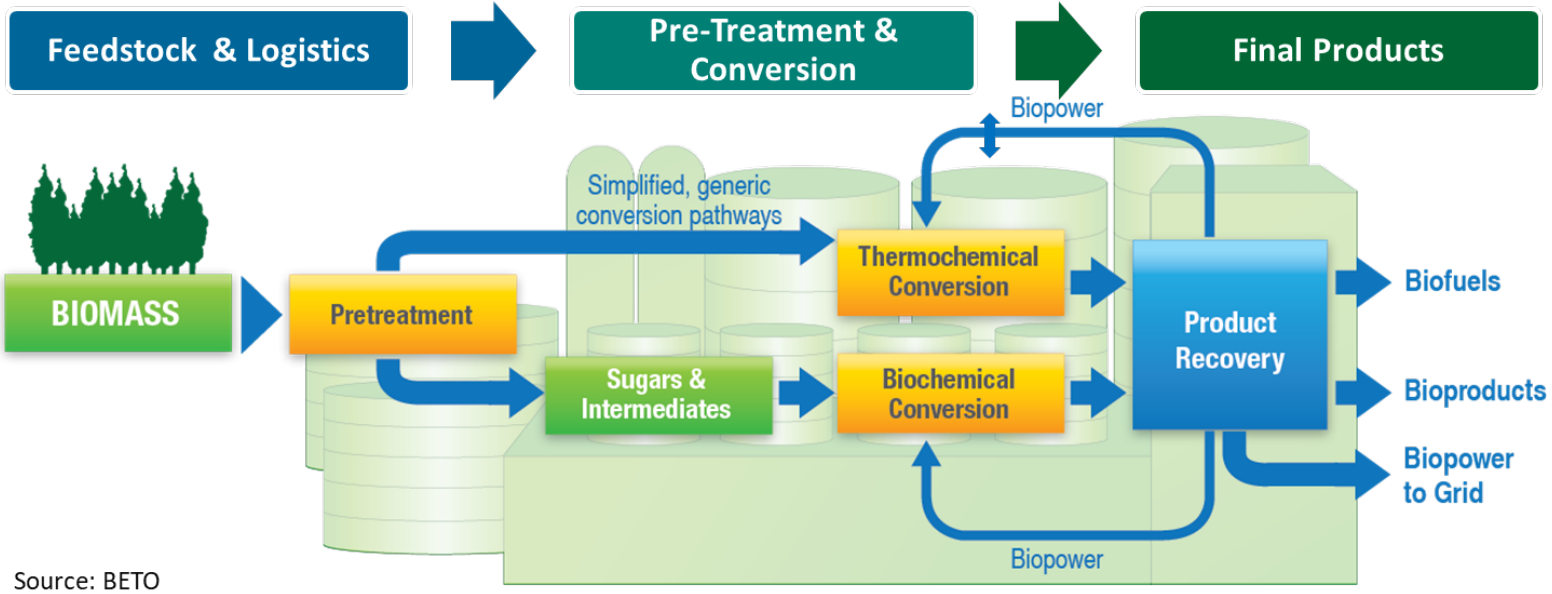
In the chemicals industry alone, improvements in catalysts and related processes could save as much as 13 exajoules of energy and 1 gigatonne of $CO_2$-equivalent per year by 2050 versus a "business-as-usual" scenario.*

*International Energy Agency, Technology Roadmap: Energy and GHG Reductions in the Chemical Industry via Catalytic Processes, 2013.

# **Project Overview:** Potential Impact of a Billion-Ton Bioeconomy



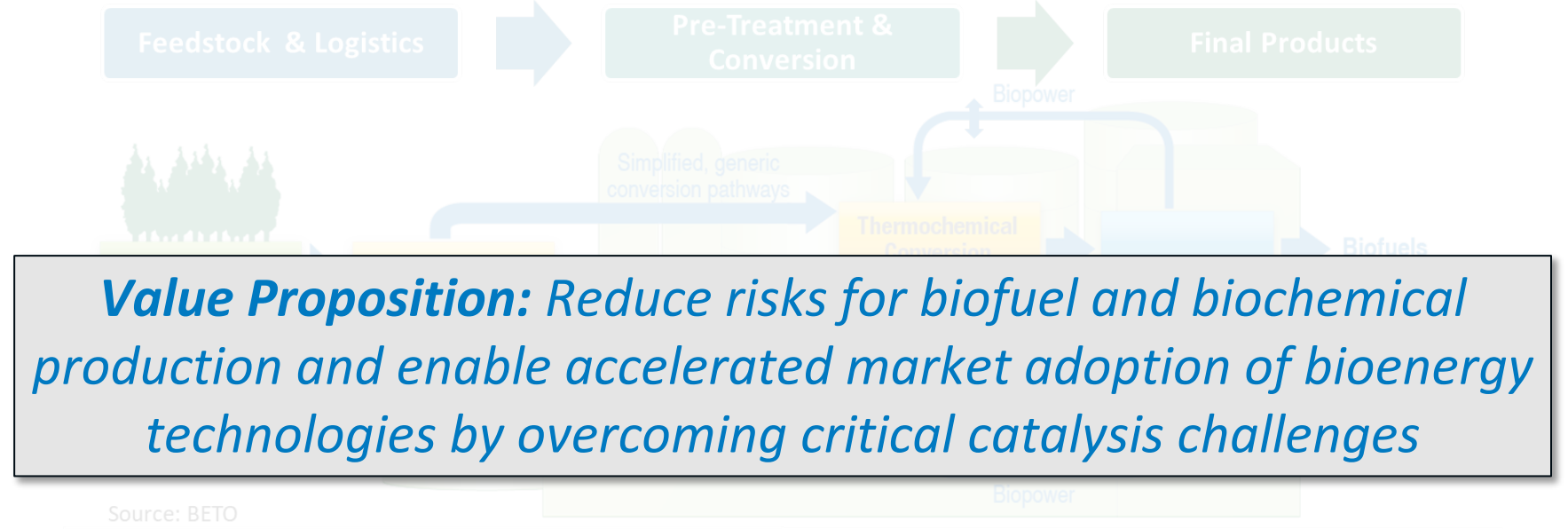
# **Project Overview:** Catalysis Challenges are Pervasive in Conversion of Biomass and Waste Feedstocks




Source: BETO

| Key Catalytic Bioenergy Processes | Challenges due to Biomass Composition |
|---|---|
| • Catalytic Upgrading of Biological Intermediates<br>• Synthesis Gas Upgrading<br>• Catalytic Fast Pyrolysis<br>• Catalytic Upgrading of Aqueous/Gaseous Waste Streams<br>• Catalytic Hydroprocessing<br>• Lignin Deconstruction and Upgrading | • High oxygen content → Broad reaction space<br>• Diverse chemical functionalities → Competing reactions<br>• High water content → Degradation of catalyst supports<br>• Impurities (S, N, alkali metals, Cl, etc.) → Poisoning<br>• Multiple states and compositions (solid, liquid, or gas)<br>• Complex, heterogeneous mixture → Difficult to model |

# **Project Overview:** Catalysis Challenges are Pervasive in Conversion of Biomass and Waste Feedstocks




***Value Proposition:*** *Reduce risks for biofuel and biochemical production and enable accelerated market adoption of bioenergy technologies by overcoming critical catalysis challenges*

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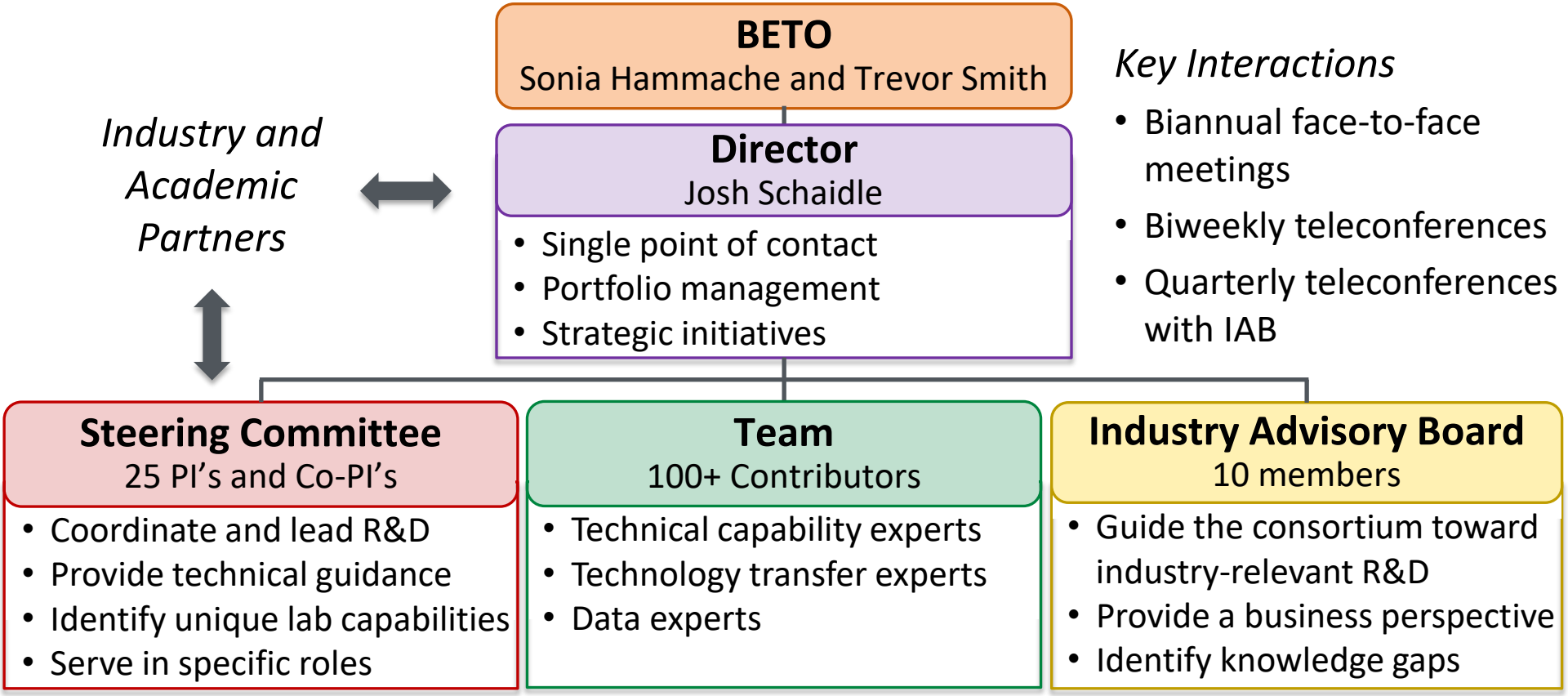
# 1. Management: Consortium Structure




**Centralized Website for Outreach: Chemcatbio.org**

# 1. Management: Communication

## *Steering Committee Roles*

**Meeting Coordination:**
Organize annual Face-to-Face and ACS Symposium


Dan Ruddy


Huamin Wang


Susan Habas


Zhenglong Li

**Industry Outreach:**
Engage with potential partners, collect feedback, and translate into action items


Mariefel Olarte


Karthi Ramasamy

**Consortia Liaison:**
Foster collaboration between BETO Consortia


Rick Elander (FCIC)


Kim Magrini (SepCon)


Derek Vardon (Co-Optima)


Jim Parks (CCPC)

**Points of Contact:**
Facilitate effective intra-consortium communication


Kurt Van Allsburg (DataHub)


Carrie Farberow


Mike Griffin (Technology Transfer)


Mark Nimlos

# 1. Management: ChemCatBio Foundation – FY19

***Integrated and collaborative portfolio of catalytic technologies and enabling capabilities***

### *Catalytic Technologies*

- **Catalytic Upgrading of Biochemical Intermediates** (NREL, PNNL, ORNL, LANL)
- **Catalytic Upgrading of Indirect Liquefaction Intermediates** (NREL, PNNL, ORNL)
- **Catalytic Fast Pyrolysis** (NREL, PNNL)
- **Electrocatalytic and Thermocatalytic $CO_2$ Utilization** (NREL, ORNL)

### *Enabling Capabilities*

- **Advanced Catalyst Synthesis and Characterization** (NREL, ANL, ORNL, SNL)
- **Catalyst Cost Model Development** (NREL, PNNL)
- **Consortium for Computational Physics and Chemistry** (ORNL, NREL, PNNL, ANL, NETL)
- **Catalyst Deactivation Mitigation for Biomass Conversion** (PNNL)

### *Industry Partnerships (Directed Funding)*

- **Gevo** (NREL)
- **ALD Nano/JM** (NREL)
- **Vertimass** (ORNL)
- **Opus12** (NREL)
- **Visolis** (PNNL)
- **Lanzatech** (PNNL) - Fuel
- **Gevo** (LANL)
- **Lanzatech** (PNNL) - TPA
- **Sironix** (LANL)

### *Cross-Cutting Support*

- **ChemCatBio Lead Team Support** (NREL)
- **ChemCatBio DataHUB** (NREL)

# 1. **Management:** Active Portfolio Management

***Integrated and collaborative portfolio of catalytic technologies and enabling capabilities***

| ***Catalytic Technologies*** | ***Enabling Capabilities*** | ***Industry Partnerships (Directed Funding)*** |
|---|---|---|
| Catalytic Upgrading of Biochemical Intermediates (NREL, PNNL, ORNL, LANL) | Advanced Catalyst Synthesis and Characterization (NREL, ANL, ORNL, SNL) | **Gevo** (NREL) |
| | | **ALD Nano/JM** (NREL) |
| **Reorganized in FY20** | **Closed out following successful tool development** | **Vertimass** (ORNL) |
| | | **Selected for Phase II** |
| Catalytic Fast Pyrolysis (NREL, PNNL) | Consortium for Computational Physics and Chemistry (ORNL, NREL, PNNL, ANL, NETL) | **Selected for Phase II** |
| | | **Lanzatech** (PNNL) - Fuel |
| **Reorganized in FY20** | **Added in FY19 based on IAB feedback** | **Gevo** (LANL) |
| | | **Lanzatech** (PNNL) - TPA |
| | | **Selected for Phase II** |

***Cross-Cutting Support***

**ChemCatBio Lead Team Support** (NREL)

**ChemCatBio DataHUB** (NREL)

# 1. **Management:** Catalytic Technologies Reorganization

***Shift projects to respond to peer review feedback and align with industry interests***

***FY19***

**Catalytic Upgrading of Indirect Liquefaction Intermediates**
(NREL, PNNL, ORNL)

**Electrocatalytic and Thermocatalytic $CO_2$ Utilization**
(NREL)

MeOH/DME Upgrading

Catalytic $CO_2$ Upgrading

***FY20***

**Upgrading of C1 Building Blocks**
(NREL)

Aligns this project with significant industrial interest in upgrading methanol, $CO_2$, and biogas

Ethanol Upgrading (PNNL/ORNL)

**Upgrading of C2 Intermediates**
(PNNL and ORNL)

Aligns this project with significant industrial interest in generating drop-in fuels and valuable chemicals from ethanol

Electrochemical $CO_2$ Upgrading

**Electrocatalytic $CO_2$ Utilization**
(NREL)

Responds to peer review feedback that project should focus on electrocatalytic $CO_2$ utilization and emphasize development and evaluation of realistic reactor (MEA) configurations

# 1. Management: ChemCatBio Foundation – FY21

***Integrated and collaborative portfolio of catalytic technologies and enabling capabilities***

### *Catalytic Technologies*

- **Catalytic Upgrading of Biochemical Intermediates** (NREL, PNNL, ORNL, LANL)
- **Upgrading of C1 Building Blocks** (NREL)
- **Upgrading of C2 Intermediates** (PNNL, ORNL)
- **Catalytic Fast Pyrolysis** (NREL, PNNL)
- **Electrocatalytic $CO_2$ Utilization** (NREL)

### *Enabling Capabilities*

- **Advanced Catalyst Synthesis and Characterization** (NREL, ANL, ORNL)
- **Consortium for Computational Physics and Chemistry** (ORNL, NREL, PNNL, ANL, NETL)
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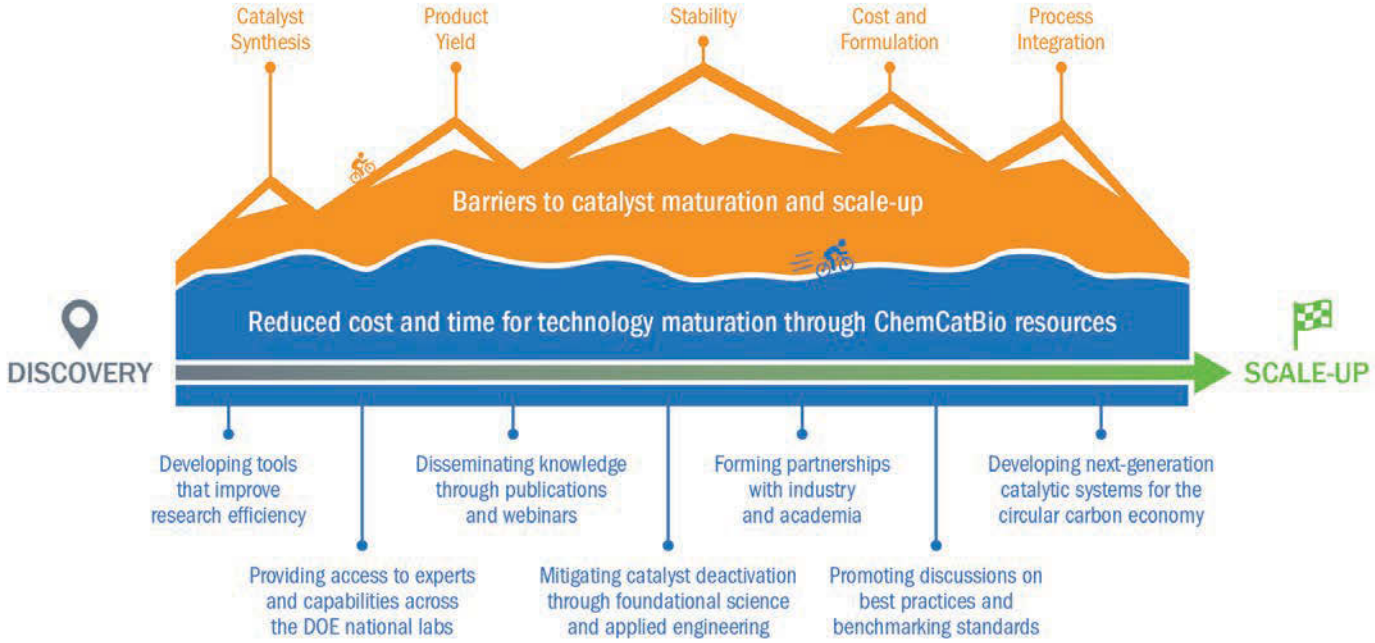
- **Opus12** (NREL)
- **Visolis** (PNNL)
- **Sironix** (LANL)

### *Cross-Cutting Support*

- **ChemCatBio Lead Team Support** (NREL)
- **ChemCatBio DataHUB** (NREL)

# 2. Approach: Acceleration

**The path to catalyst deployment is slow and difficult.**




**ChemCatBio is accelerating the catalyst and process development cycle.**

# 2. Approach: Foundational Catalyst-Process R&D

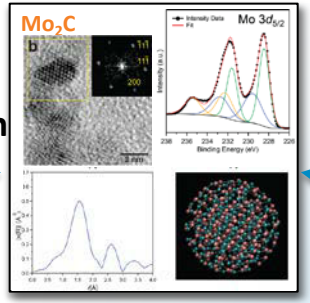
***Foundational Science***

*Enables hypothesis-driven catalyst design*

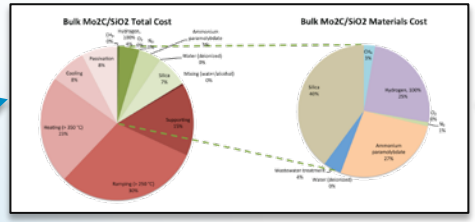
***Applied Engineering***

*Enables evaluation of key process metrics and deactivation*

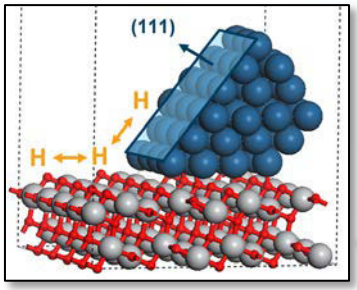
**Advanced Synthesis and Characterization**



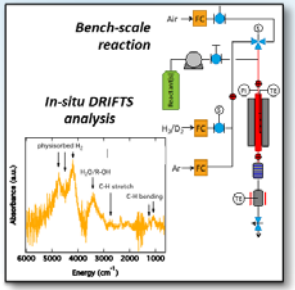

**Catalyst Cost Estimation (CatCost™)**

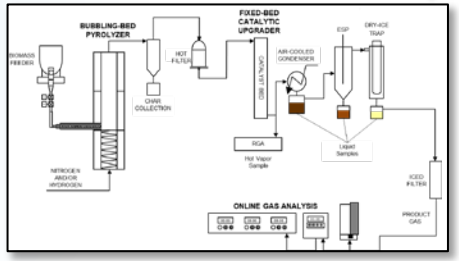



**Theory**




**Performance Evaluation**




**Catalyst Scaling and Integrated Testing**

# 2. Approach: Differentiators

***Value Proposition:*** *Reduce risks for biofuel and biochemical production and enable accelerated market adoption of bioenergy technologies by overcoming critical catalysis challenges*

***Differentiators:***

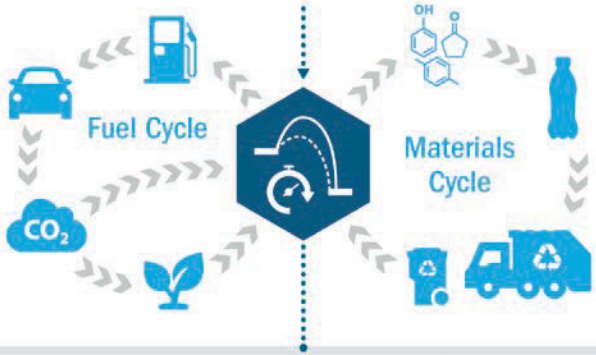
- Working with realistic process streams (woody biomass, fermentation broth)
- Targeting both pathway-specific and overarching catalysis challenges
  - Emphasis on mitigating catalyst deactivation as a grand challenge
- Leveraging world-class national lab capabilities and expertise
- Guiding R&D through risk assessment, technoeconomic analysis/life-cycle assessment and input from our industry advisory board
- Advancing core catalytic upgrading technologies for BETO

# **3. Impact:** Serving as a Central Hub of Knowledge

Addressing ***critical catalysis challenges*** limiting commercialization of bioenergy technologies and ***facilitating industry access*** to national lab capabilities and expertise

Catalysis enables a circular carbon economy.

**85% of industrial chemical processes rely on catalysts.**




**ChemCatBio** is accelerating catalyst development for bioenergy applications:

**SCIENTIFIC CONTRIBUTIONS**

**>135** publications

**34** h-index since 2016

**>2,800** citations

**1** R&D100 Special Recognition

**THE TEAM**

**>130** researchers

**8** DOE National Labs

**BETO** -sponsored

**14** Industry Advisory Board Members

**MARKET IMPACT**

**3** technology licenses

**1** software copyright

**27** issued patents and patent applications

**12** awarded projects with industry

**COMMUNITY RESOURCES**

**3 enabling tools** CatCost, Catalyst Property Database, Surface Phase Explorer

**9** webinars

Directed Funding Opportunities for industry

Streamlined access to unique national lab capabilities

**Maintain an updated website to facilitate community outreach: Chemcatbio.org**

# 3. **Impact:** Path to Market

Addressing ***critical catalysis challenges*** limiting commercialization of bioenergy technologies and ***facilitating industry access*** to national lab capabilities and expertise

- 3 ChemCatBio technologies licensed by industry
  - Ethanol to jet fuel
  - Dimethyl ether to high-octane gasoline
  - Atomic Layer Deposition
- Multiple follow-on projects with industry (TCF, FOA, CRADA)
- Successfully completed Phase I Directed Funding Opportunities
  - R&D100 Special Recognition in Green Tech (Sironix)
  - Gevo: "The insight provided by ChemCatBio through ***advanced characterization techniques that are not readily available to industry*** has helped us to develop a better understanding of catalyst deactivation for important Gevo biofuels processes."
- FY20 CatCost™ Utilization: 1,492 users / 2,077 sessions

# 4. **Progress:** Addressing Catalyst Deactivation

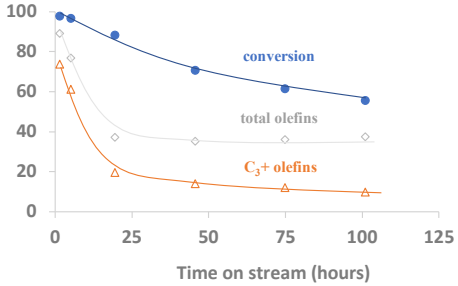
## Catalyst deactivation is a critical risk for commercialization of bioenergy applications

### Ethanol Upgrading

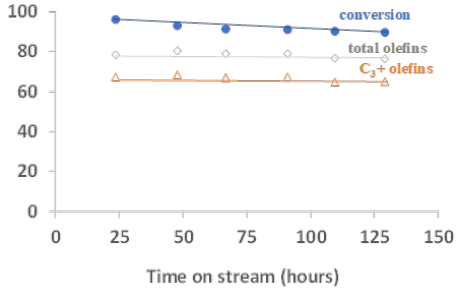
***Challenge:*** Coke formation

***Accomplishment:*** 3x reduction in coke formation through catalyst modification, resulting in enhanced stability

FY19



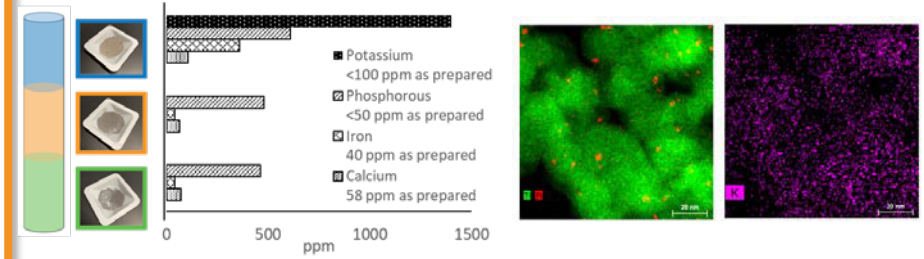

FY20

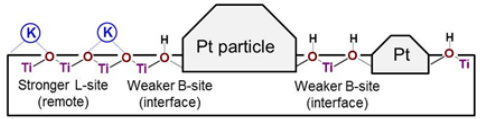



### Catalytic Fast Pyrolysis

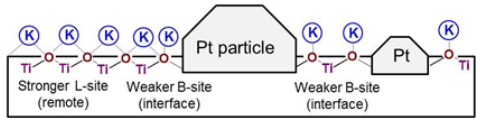
***Challenge:*** Potassium deposition

***Accomplishment:*** Developed a mechanistic understanding of K-induced deactivation through comprehensive catalyst characterization and testing




Low K loading



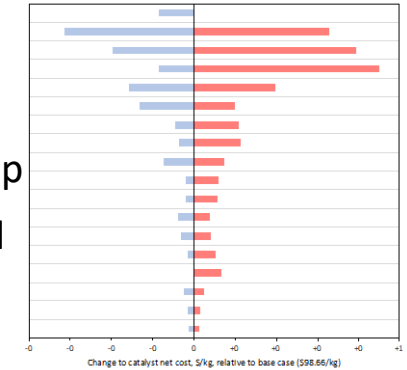

High K loading

# 4. **Progress:** Tool Development

Expanding the development and utilization of tools that improve research efficiency and accelerate the catalyst-process development cycle

## Enhanced capabilities of CatCost™

- Added Python scripts for Web-Excel interconversion
- Created printable outputs in Excel to support peer review
- Incorporated sensitivity analysis into the Web App
- Fixed bugs and improved performance




catcost.chemcatbio.org

## Developed and publicly released the Catalyst Property Database

- Centralized, searchable compilation of published density functional theory adsorption data
- Standardization of 3000+ datapoints through development and implementation of dictionaries
- Key component of the Catalyst Design Engine

### Catalyst Design Engine Vision


cpd.chemcatbio.org

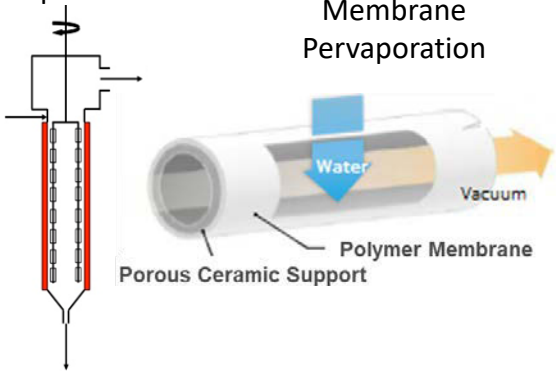
# 4. **Progress:** Engagement with other Consortia

Rich cross-consortia collaboration enables broader impact to the bioenergy community

## Improving efficiency of butanediol upgrading through advanced separations

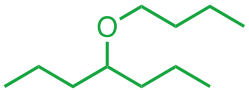
Wiped Film Evaporation

Membrane Pervaporation




BIOPROCESSING SEPARATIONS CONSORTIUM

## Producing diesel blendstocks through catalytic upgrading of short-chain acids

4-Butoxyheptane

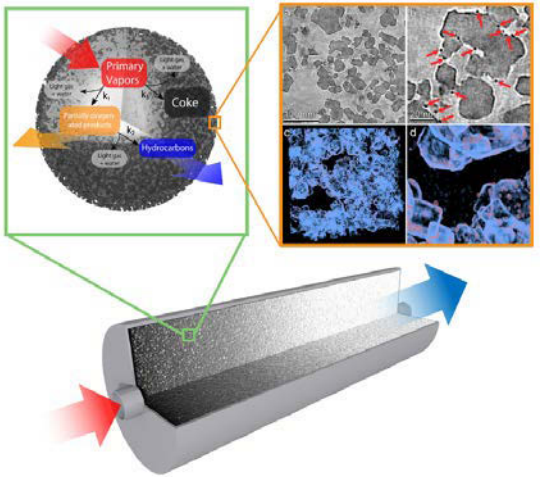
5-Ethyl-4-Propylnonane

X. Huo, et al., *Green Chem.* 21 (2019) 5813-5827.

G. Hafenstine, et al., *Green Chem.* 22 (2020) 4463-4472.

Co-Optimization of Fuels & Engines

## Informing catalyst and process scale-up for CFP




M. Pecha, et al., *React. Chem. Eng.* 6 (2021) 125-137

CCPC Consortium for Computational Physics and Chemistry

U.S. DEPARTMENT OF ENERGY BIOENERGY TECHNOLOGIES OFFICE

# 4. **Progress:** Industry and Stakeholder Engagement

## Industry engagement and partnerships help maintain commercial relevance

### Revamped our Industry Advisory Board in 2020 to bring in new perspectives

- 10 members across the catalysis and bioenergy value chains
- Expanded to include academic members
- Members from Phillips66, W.R. Grace, Clariant, JohnsonMatthey, ExxonMobil, Columbia University, and Apeel Sciences
- Quarterly meetings

### Initiated 3 Phase II industrial partnerships through Directed Funding Opportunity

VISOLIS CARBON NEGATIVE MATERIALS

SIRONIX RENEWABLES

OPUS 12

- Building off success from Phase I projects to facilitate commercial impact
- Leveraging ChemCatBio capabilities in synthesis, characterization, and evaluation
- Advancing technology readiness level

### Interviewed subject matter experts to guide ChemCatBio's evolution as a "Central Hub of Knowledge"

- Prior listening day feedback suggested ChemCatBio serve as a "Central Hub of Knowledge"
- Interviewed >25 industry experts to understand knowledge gaps and needs
- ***Outcome:*** Identified specific action items, including newsletter distribution and SOT updates through our website

# Summary

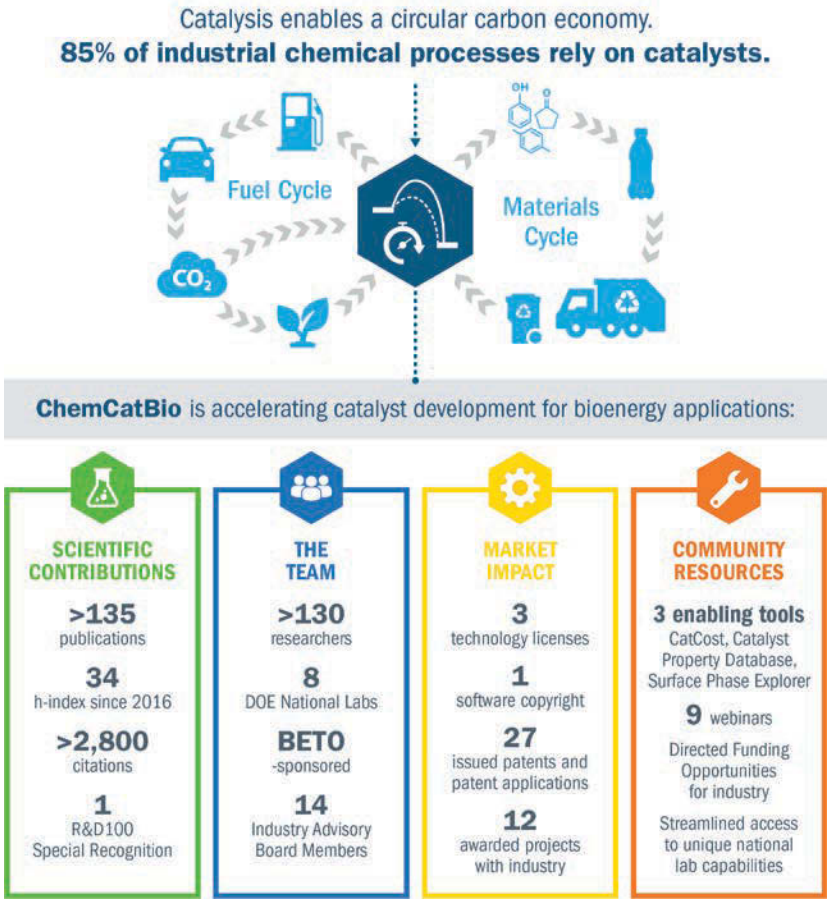
**Mission:** Accelerate the catalyst and process development cycle for bioenergy applications

**Approach:** Active consortium management combined with a ***collaborative R&D*** approach guided by risks, TEA/LCA, and stakeholder/IAB input that targets both pathway-specific and overarching catalysis challenges

- Developing next-generation catalytic systems
- Mitigating deactivation
- Developing tools that improve research efficiency
- Establishing partnerships & disseminating knowledge

**Outcome:** Reduced cost, time, and risks for catalytic technology maturation

**Relevance to Bioenergy Industry:** Addressing ***critical catalysis challenges*** limiting commercialization of bioenergy technologies and ***facilitating industry access*** to national lab capabilities and expertise



# Acknowledgements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Energy Materials Network
U.S. Department of Energy

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BIOENERGY TECHNOLOGIES OFFICE

**Steering Committee**

Rajeev Assary (ANL)
Fred Baddour (NREL)
Rob Dagle (PNNL)
Vanessa Dagle (PNNL)
Rick Elander (NREL)
Carrie Farberow (NREL)
Jack Ferrell (NREL)
Mike Griffin (NREL)
Susan Habas (NREL)
David Johnson (NREL)
Ted Krause (ANL)
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Kim Magrini (NREL)
Cameron Moore (LANL)
Mariefel Olarte (PNNL)
Asanga Padmaperuma (PNNL)
Jim Parks (ORNL)
Karthi Ramasamy (PNNL)
Roger Rousseau (PNNL)
Dan Ruddy (NREL)
Andrew Sutton (ORNL)
Madhava Syamlal (NETL)
Kinga Unocic (ORNL)
Kurt Van Allsburg (NREL)
Derek Vardon (NREL)
Huamin Wang (PNNL)

**BETO**

Sonia Hammache
Trevor Smith
Nichole Fitzgerald
Andrea Bailey
Kevin Craig

**Special thanks to all of our collaborators and industry advisory board members!**

# Thank you!


## ChemCatBio Team

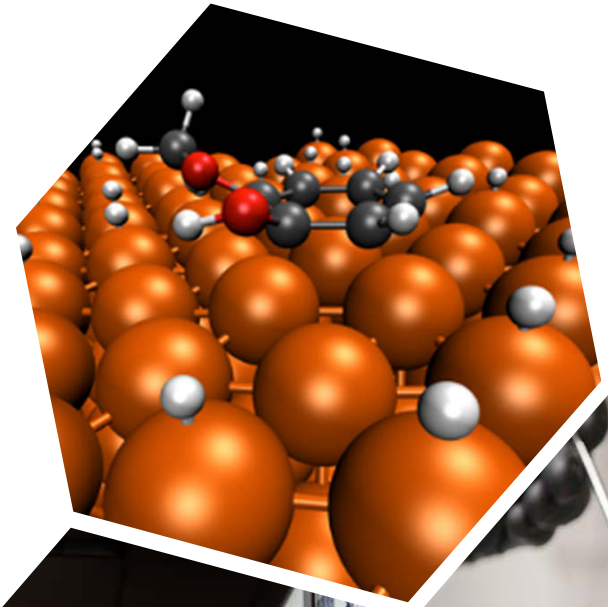
ChemCatBio
Chemical Catalysis for Bioenergy

DOE Bioenergy Technologies Office (BETO) 2021 Project Peer Review

# Overview of the Chemical Catalysis for Bioenergy Consortium

March 9th, 2021
Catalytic Upgrading

Josh Schaidle



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# Quad Chart Overview – ChemCatBio Lead Team Support (WBS 2.6.3.500)

## Timeline

- Start Date: October 1st, 2019
- End Date: September 30th, 2022

| | FY20 | Active Project |
|---|---|---|
| **DOE Funding** | $160,000 | $480,000 |

## Barriers addressed

***Ot-B: Cost of Production***
Reducing conversion cost contribution to MFSP

***Ct-E/F: Improving yield and catalyst lifetime***
Developing stable, selective catalysts

***Ct-G: Decreasing time/cost to develop catalysts***
Leverage national lab capabilities/expertise

## Project Goal

Enable ChemCatBio to achieve its mission by providing leadership for the consortium, managing the R&D portfolio, serving as single point of contact for potential partners, pursuing action items identified from the stakeholder listening day, and developing strategic initiatives to position the consortium for the future.

## End of Project Milestone

Establish ChemCatBio as a central public hub of knowledge, methods, and tools for catalytic bioenergy applications by (1) supporting development of the Catalyst Design Engine (including release of a computational catalyst database web application), (2) maintaining and expanding the capabilities of the CatCost tool, (3) developing and sharing content on our website about mitigation of catalyst deactivation, advancements in the state-of-technology for applicable conversion pathways, and the catalyst value factor, and (4) implementing action items based on feedback from the community in FY20.

## Funding Mechanism

Annual Operating Plan (AOP)

# Acknowledgement

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# Additional Slides

# Responses to Previous Reviewers' Comments

Our overarching response to 2019 peer review feedback:

"Moving forward, we will continue to build upon the collaborative foundation of the consortium and our early-stage technical successes by (1) maintaining our responsiveness to stakeholder feedback, (2) emphasizing carbon utilization as a key metric for all catalytic conversion technologies, (3) strengthening existing partnerships and developing new partnerships, especially with industry and other BETO consortia (e.g., Separations Consortium), and (4) developing tools that broadly enable the research community to accelerate the catalyst and process development cycle for bioenergy technologies."

# Publications, Patents, Presentations, Awards, and Commercialization

- Full list of ChemCatBio Publications: https://www.chemcatbio.org/publications.html
- Full list of ChemCatBio Webinars: https://www.chemcatbio.org/webinars.html
- See slides 15 and 16 regarding awards, patents, licenses, and industry collaborations

# **Project Overview:** Historical Motivation

2015 PROJECT PEER REVIEW
U.S. DEPARTMENT OF ENERGY
BIOENERGY TECHNOLOGIES OFFICE

Energy Materials Network
U.S. Department of Energy

***Feedback:*** *Establish an "Experimental Catalysis Consortium"*

- Address *overarching issues* such as deactivation and physical stability
- Needs to be a *highly-coordinated* effort focused on *advancing the state of technology for catalysis*, not just pathway-specific challenges
- Integrate *valorization of waste streams*

***Goal:*** *Accelerate the development of advanced materials for clean energy applications*

- Consists of national lab-led *consortia*
- Integrates all phases of R&D from *discovery to scale-up*
- Facilitates *industry/stakeholder access* to a world-class network of capabilities, tools, and expertise

ChemCatBio
Chemical Catalysis for Bioenergy

[Launched at start of FY17]