

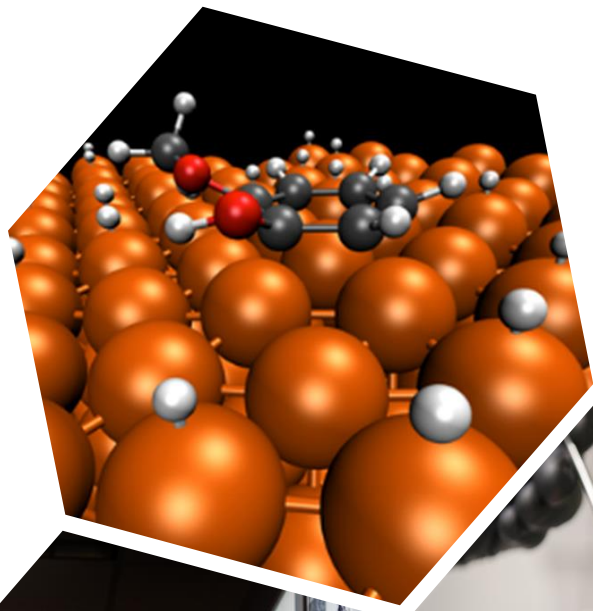


DOE Bioenergy Technologies Office (BETO) 2021 Project Peer Review

Overview of the Chemical Catalysis for Bioenergy Consortium

March 9th, 2021
Catalytic Upgrading

Josh Schaidle



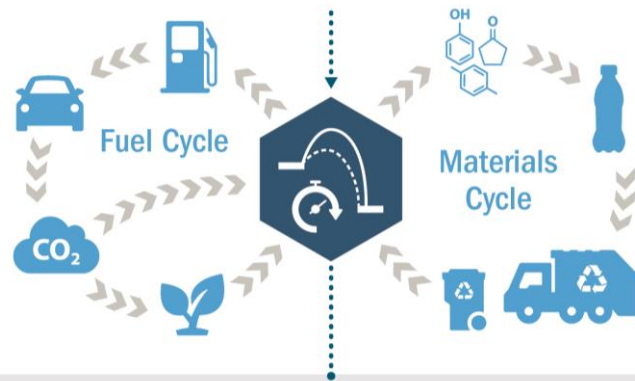
Project Overview: ChemCatBio Mission

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

Vision: A rapid transition to a circular carbon economy

Catalysis enables a circular carbon economy.

85% of industrial chemical processes rely on catalysts.



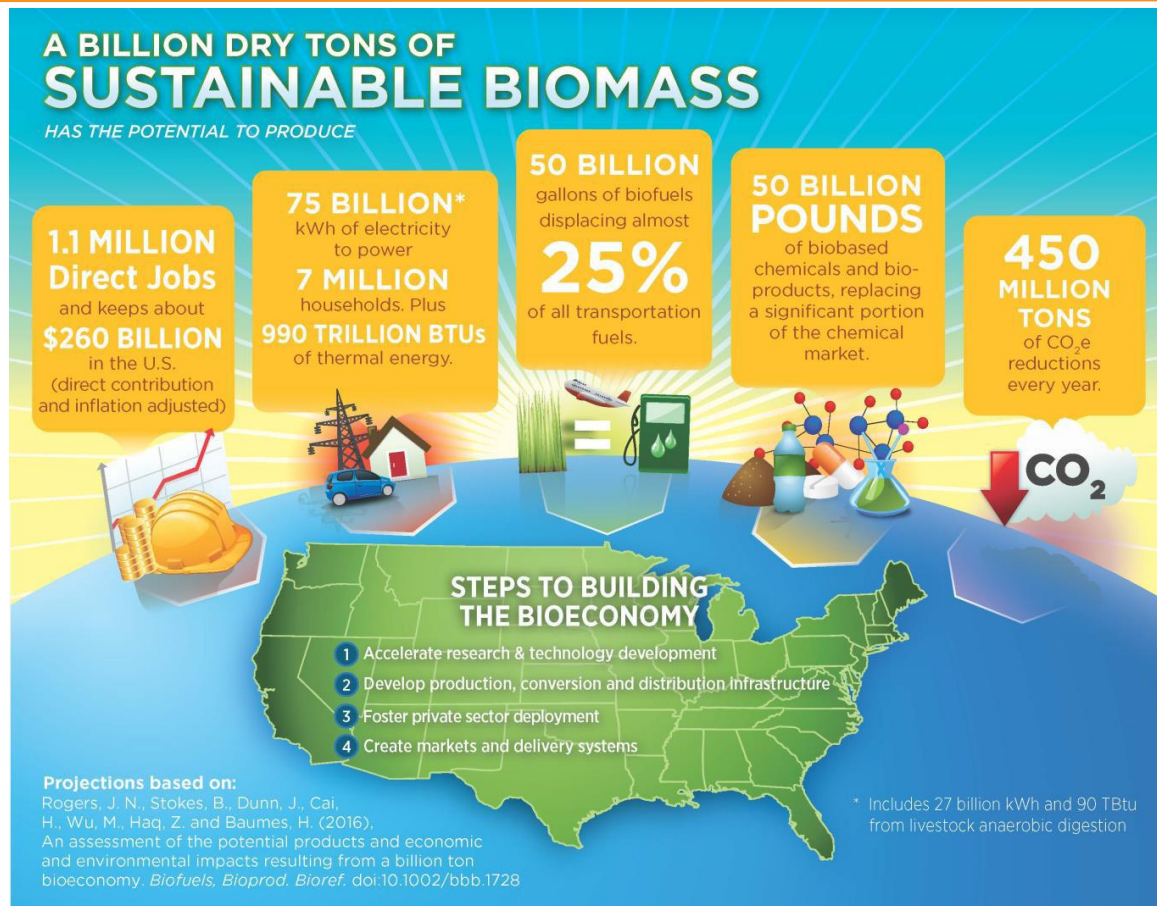
ChemCatBio is accelerating catalyst development for bioenergy applications

Potential Future Impact of Catalysis

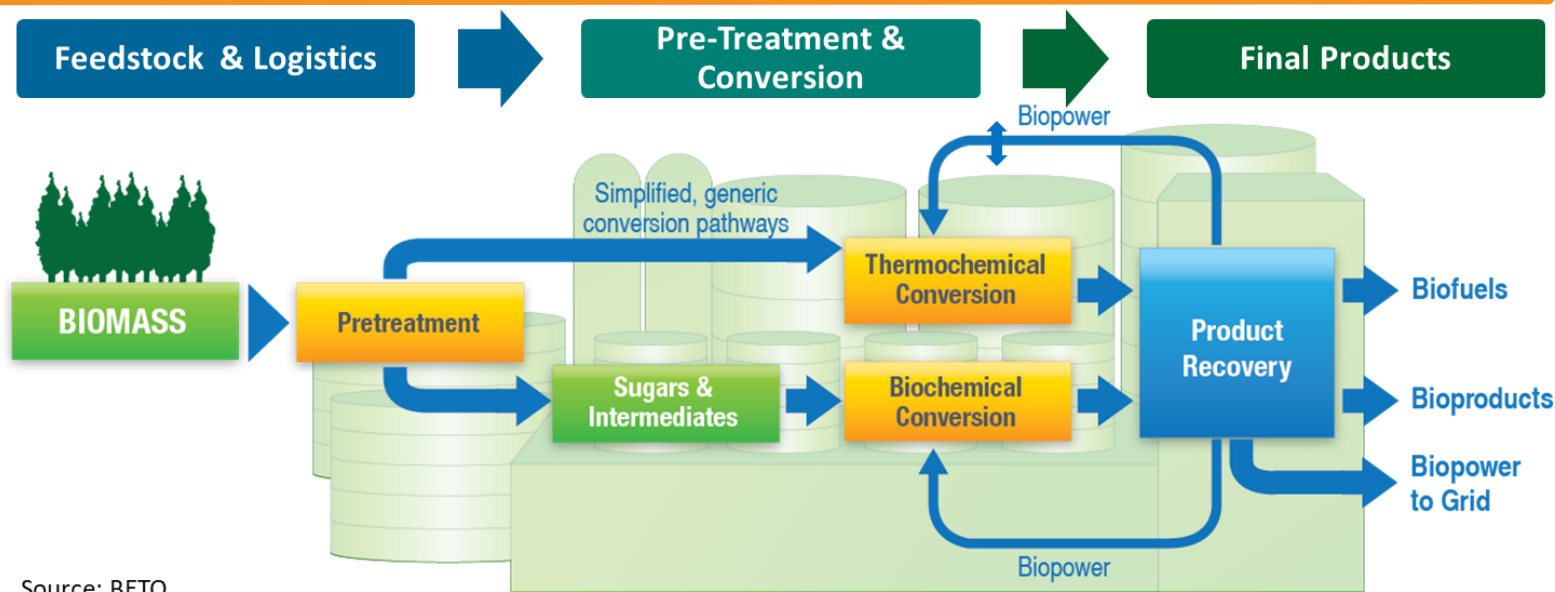
In the chemicals industry alone, improvements in catalysts and related processes could save as much as 13 exajoules of energy and 1 gigatonne of CO₂-equivalent per year by 2050 versus a “business-as-usual” scenario.*

*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

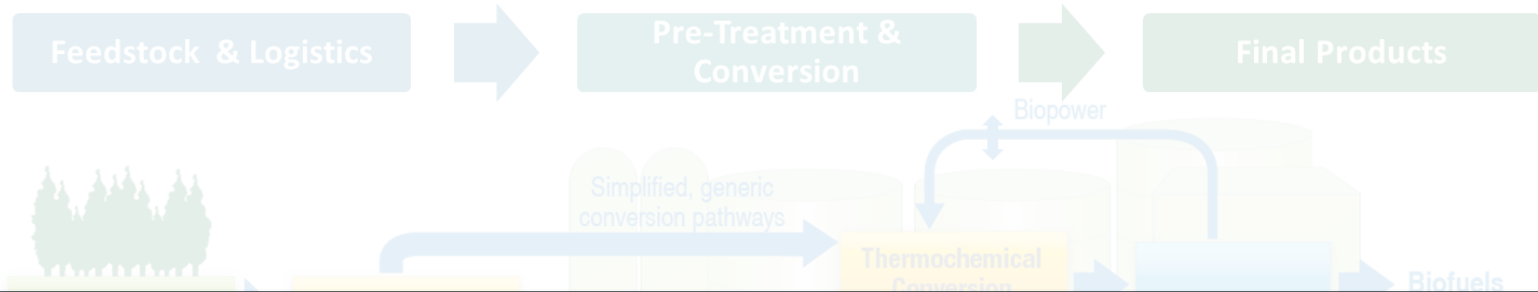
Key Catalytic Bioenergy Processes

- Catalytic Upgrading of Biological Intermediates
- Synthesis Gas Upgrading
- Catalytic Fast Pyrolysis
- Catalytic Upgrading of Aqueous/Gaseous Waste Streams
- Catalytic Hydroprocessing
- Lignin Deconstruction and Upgrading

Challenges due to Biomass Composition

- High oxygen content → Broad reaction space
- Diverse chemical functionalities → Competing reactions
- High water content → Degradation of catalyst supports
- Impurities (S, N, alkali metals, Cl, etc.) → Poisoning
- Multiple states and compositions (solid, liquid, or gas)
- Complex, heterogeneous mixture → Difficult to model

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

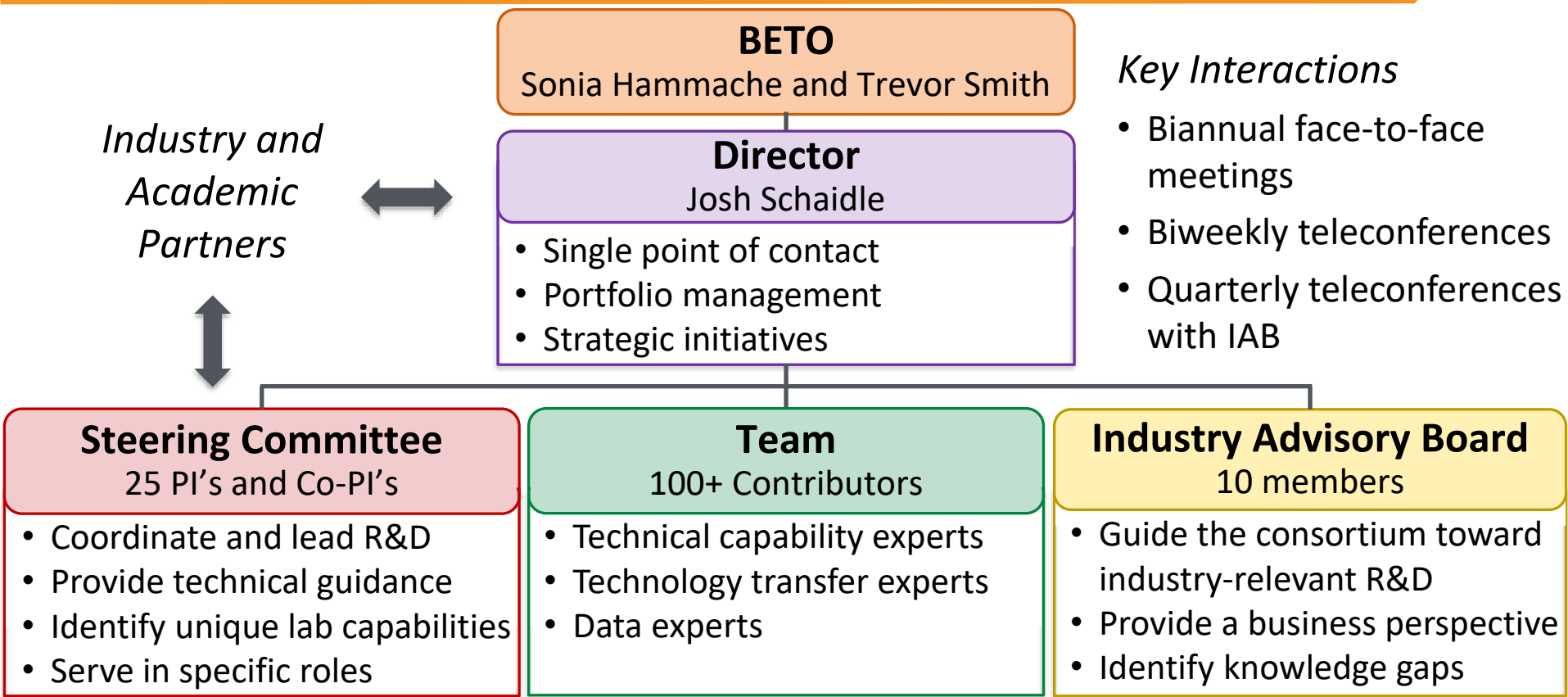


Value Proposition: Reduce risks for biofuel and biochemical production and enable accelerated market adoption of bioenergy technologies by overcoming critical catalysis challenges

Source: BETO

Key Catalytic Bioenergy Processes	Challenges due to Biomass Composition
<ul style="list-style-type: none">• Catalytic Upgrading of Biological Intermediates• Synthesis Gas Upgrading• Catalytic Fast Pyrolysis• Catalytic Upgrading of Aqueous/Gaseous Waste Streams• Catalytic Hydroprocessing• Lignin Deconstruction and Upgrading	<ul style="list-style-type: none">• High oxygen content → Broad reaction space• Diverse chemical functionalities → Competing reactions• High water content → Degradation of catalyst supports• Impurities (S, N, alkali metals, Cl, etc.) → Poisoning• Multiple states and compositions (solid, liquid, or gas)• Complex, heterogeneous mixture → Difficult to model

1. Management: Consortium Structure



Centralized Website for Outreach: [Chemcatbio.org](https://chemcatbio.org)

1. Management: Communication

Steering Committee Roles

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



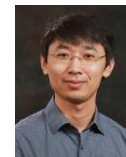
Dan Ruddy



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



Carrie Farberow
(DataHub)



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 CO₂ 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)

Vertimass (ORNL)

Reorganized in FY20

Closed out following successful tool development

Selected for Phase II

Selected for Phase II

Catalytic Fast Pyrolysis
(NREL, PNNL)

Consortium for Computational Physics and Chemistry
(ORNL, NREL, PNNL, ANL, NETL)

Lanzatech (PNNL) - Fuel

Gevo (LANL)

Lanzatech (PNNL) - TPA

Reorganized in FY20

Added in FY19 based on IAB feedback

Selected for Phase II

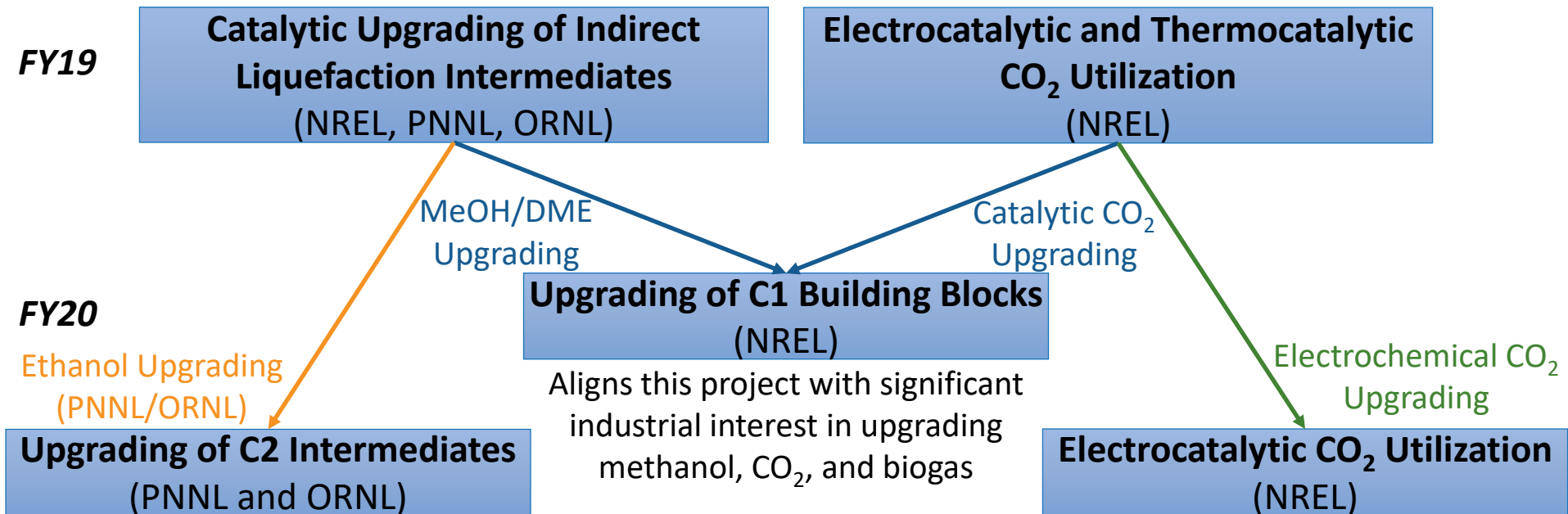
Cross-Cutting Support

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



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

Responds to peer review feedback that project should focus on electrocatalytic CO₂ 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 CO₂ Utilization
(NREL)

Enabling Capabilities

Advanced Catalyst Synthesis and Characterization
(NREL, ANL, ORNL)

Consortium for Computational Physics and Chemistry
(ORNL, NREL, PNNL, ANL, NETL)

Catalyst Deactivation Mitigation for Biomass Conversion
(PNNL)

Industry Partnerships (Phase II Directed Funding)

Opus12 (NREL)

Visolis (PNNL)

Sironix (LANL)

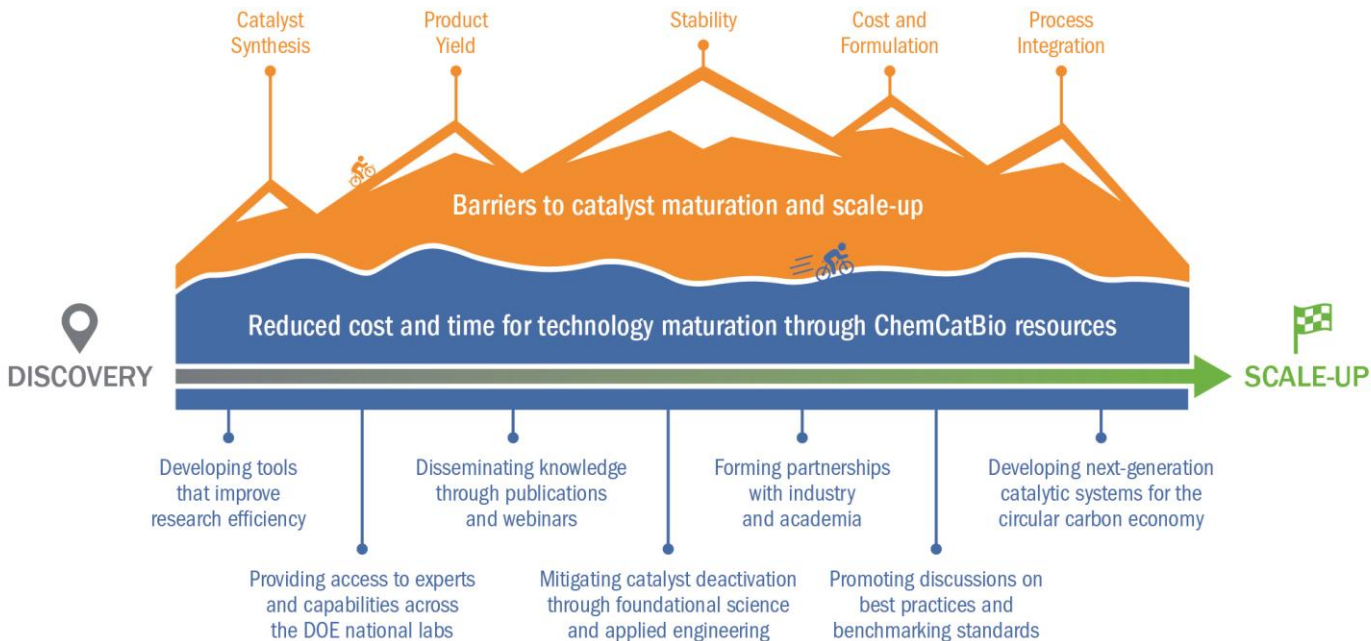
Cross-Cutting Support

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

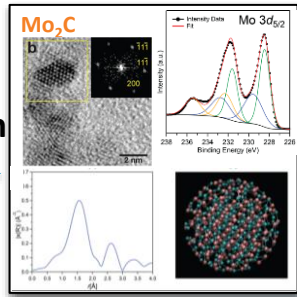
Foundational Science

Enables hypothesis-driven catalyst design

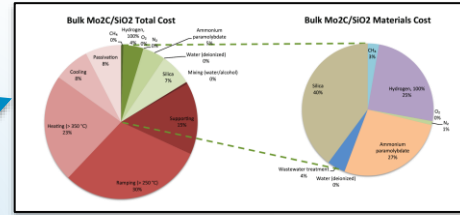
Applied Engineering

Enables evaluation of key process metrics and deactivation

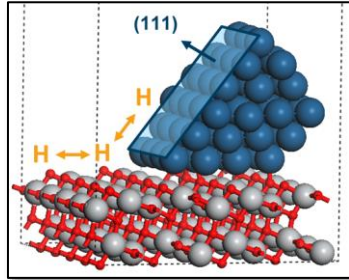
Advanced Synthesis and Characterization



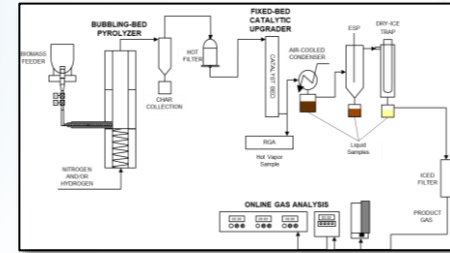
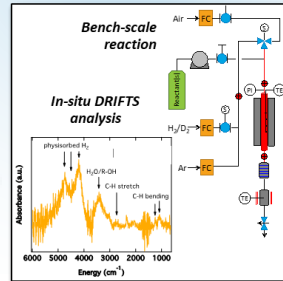
Catalyst Cost Estimation (CatCost™)



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

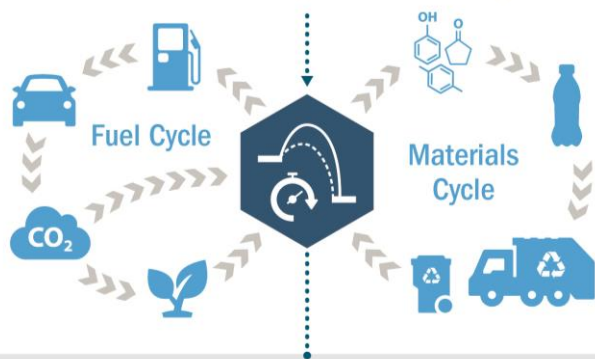
Differentiators:

- 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, techno-economic 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](https://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

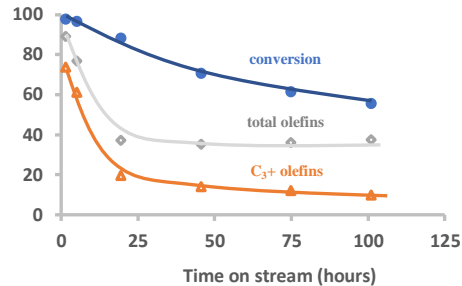
Catalyst deactivation is a critical risk for commercialization of bioenergy applications

Ethanol Upgrading

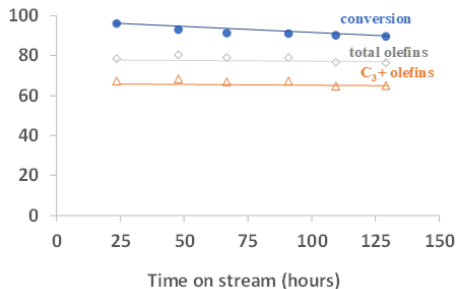
Challenge: Coke formation

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

FY19



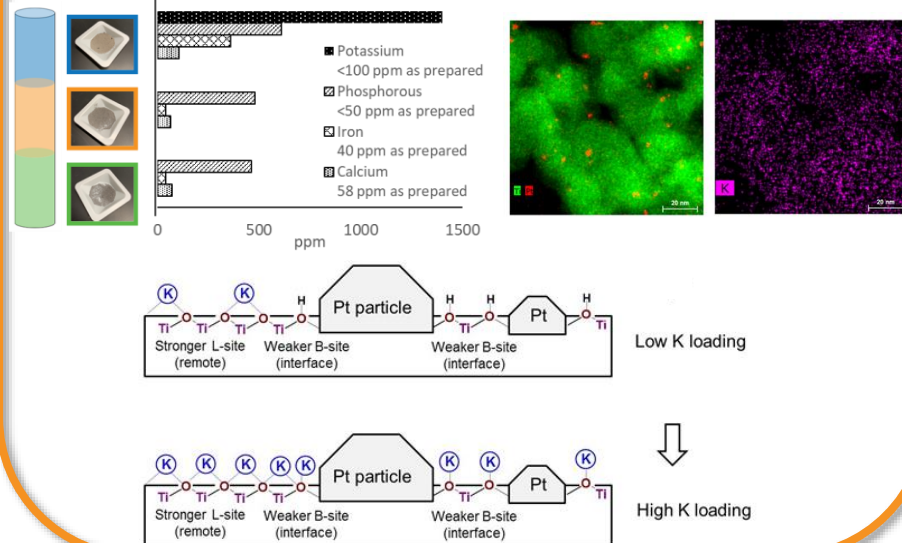
FY20



Catalytic Fast Pyrolysis

Challenge: Potassium deposition

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

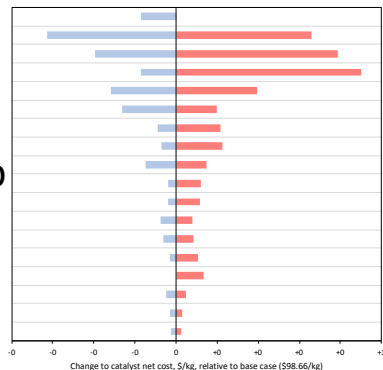


4. Progress: Tool Development

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



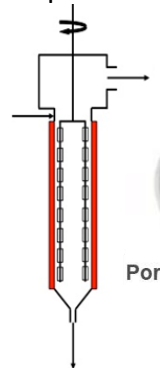
cpd.chemcatbio.org

4. Progress: Engagement with other Consortia

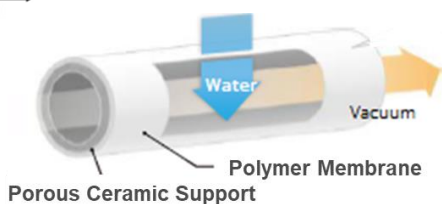
Rich cross-consortia collaboration enables broader impact to the bioenergy community

Improving efficiency of butanediol upgrading through advanced separations

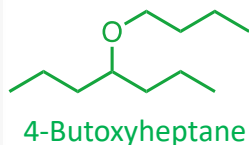
Wiped Film Evaporation



Membrane Pervaporation



Producing diesel blendstocks through catalytic upgrading of short-chain acids

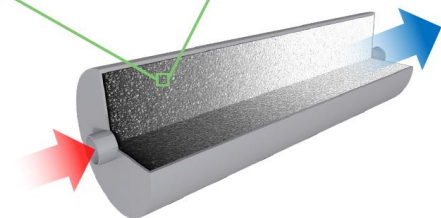
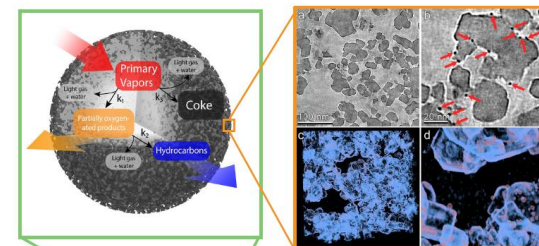


X. Huo, et al., *Green Chem.* 21 (2019) 5813-5827.

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



Informing catalyst and process scale-up for CFP



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



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



- 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

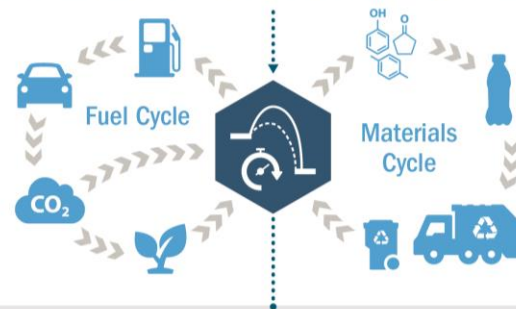
Approach: Active consortium management combined with a **collaborative R&D** approach guided by risks, TEA/LCA, and stakeholder/IAB input that targets both pathway-specific and overarching catalysis challenges

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

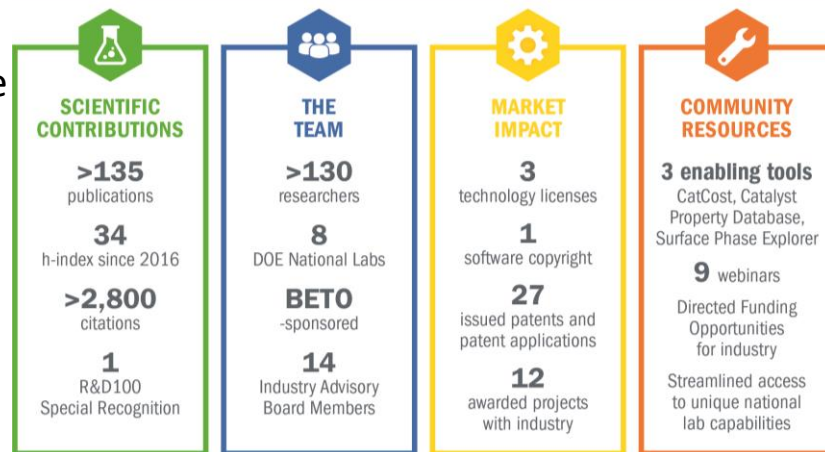
Outcome: Reduced cost, time, and risks for catalytic technology maturation

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

Catalysis enables a circular carbon economy.
85% of industrial chemical processes rely on catalysts.



ChemCatBio is accelerating catalyst development for bioenergy applications:



Acknowledgements



Energy Materials Network

U.S. Department of Energy



Office of **ENERGY EFFICIENCY
& RENEWABLE ENERGY**

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)

Zhenglong Li (ORNL)

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

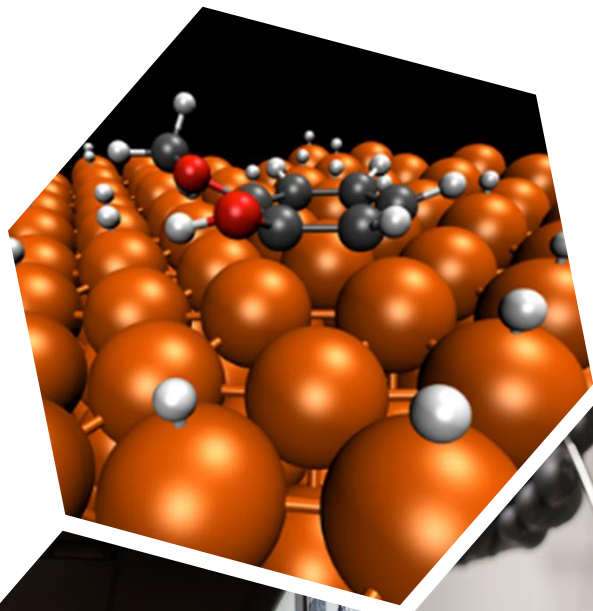


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Overview of the Chemical Catalysis for Bioenergy Consortium

March 9th, 2021
Catalytic Upgrading

Josh Schaidle



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)

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

