ChemCatBio
Chemical Catalysis for Bioenergy

Pursuing the rapid decarbonization of our economy

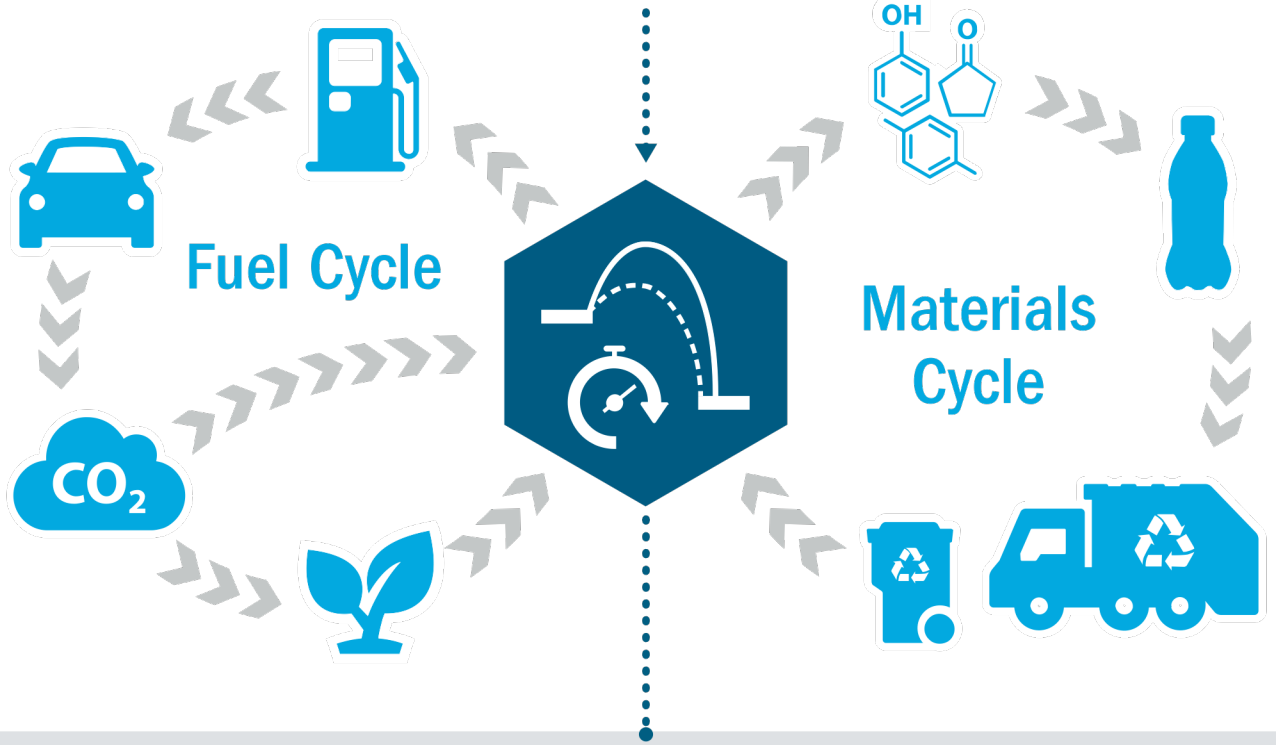
Accelerating the catalyst and process development cycle for bioenergy applications

Joshua Schaidle, Director
Daniel Ruddy, Deputy Director
April 2023

Overview: Catalysis for 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

Overview: Biomass for the SAF Grand Challenge

Could grow more than 1 billion tons per year of biomass

-Sustainably harvested in the US for biofuel (not competing with food)

U.S. Department of Energy. 2016. *2016 Billion-Ton Report: Advancing Domestic Resources for a Thriving Bioeconomy*.

Dept. of Energy's Sustainable Aviation Fuel (SAF) Grand Challenge

- Minimum 50% reduction in life cycle greenhouse gas (GHG) emissions vs petro-jet
- Meet 100% of aviation fuel demand by 2050
- Catalysis is required in **every** approved ASTM pathway

Photo courtesy of istock.com

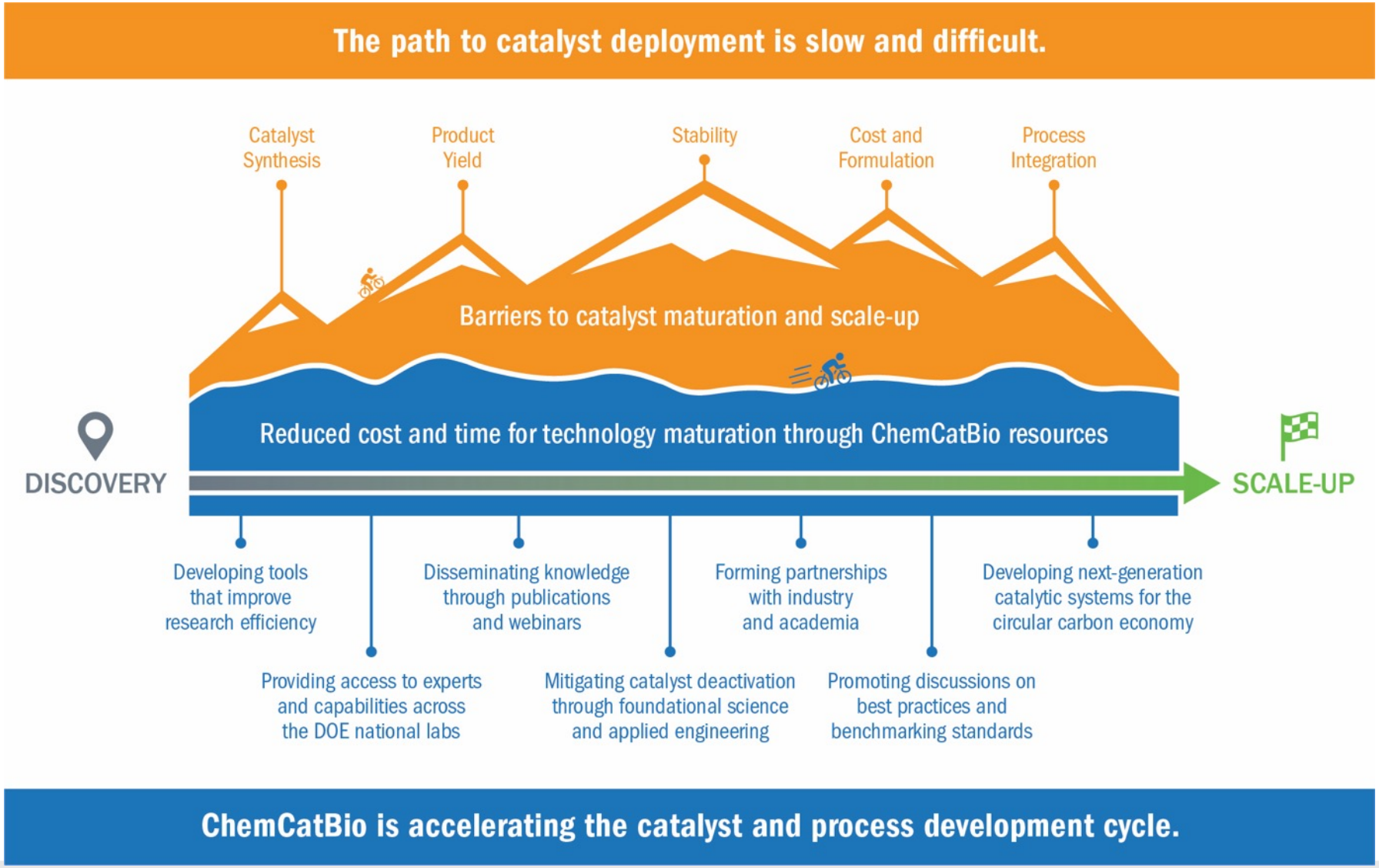
https://www.energy.gov/eere/bioenergy/sustainable-aviation-fuel-grand-challenge

How much SAF can we get from all that biomass?

- At 50 gal/ton = 50 billion gal/year, exceeding current demand (21 Bgal/year)
  - Compatible with ***existing infrastructure***

Approach: Reducing the Height of the Barriers to Success

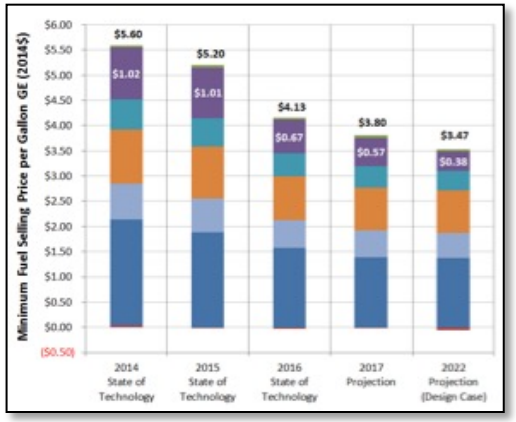
A major part of ChemCatBio's mission is providing resources that accelerate R&D



Approach: Dual Cycle for Catalyst & Process R&D

Synthesis & Characterization

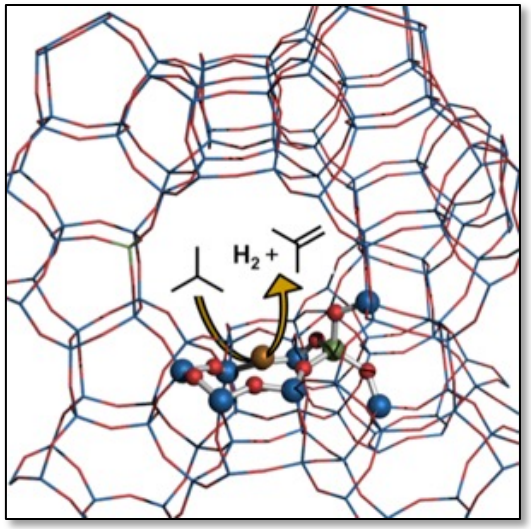
Techno-Economic and Life-Cycle Analyses (TEA, LCA)



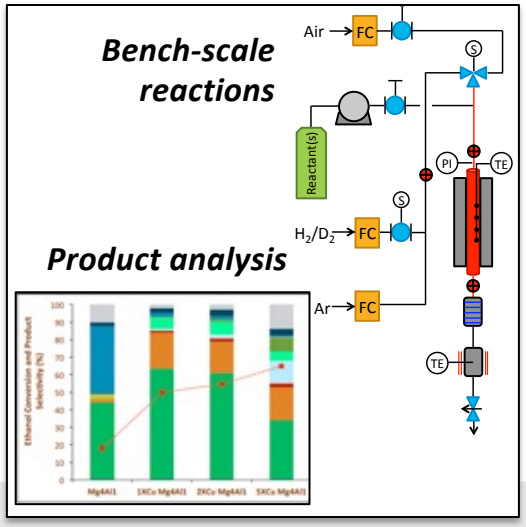
Foundational Catalysis Science

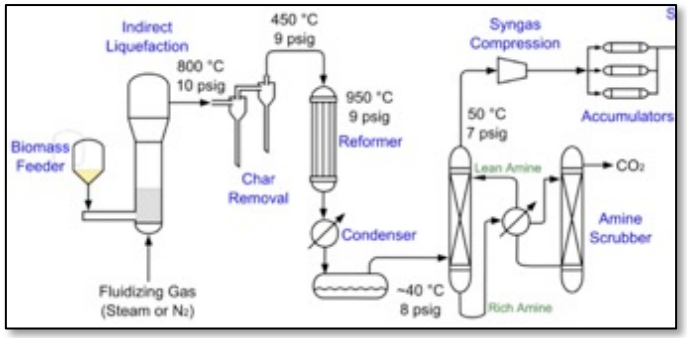
Applied Engineering

Computation



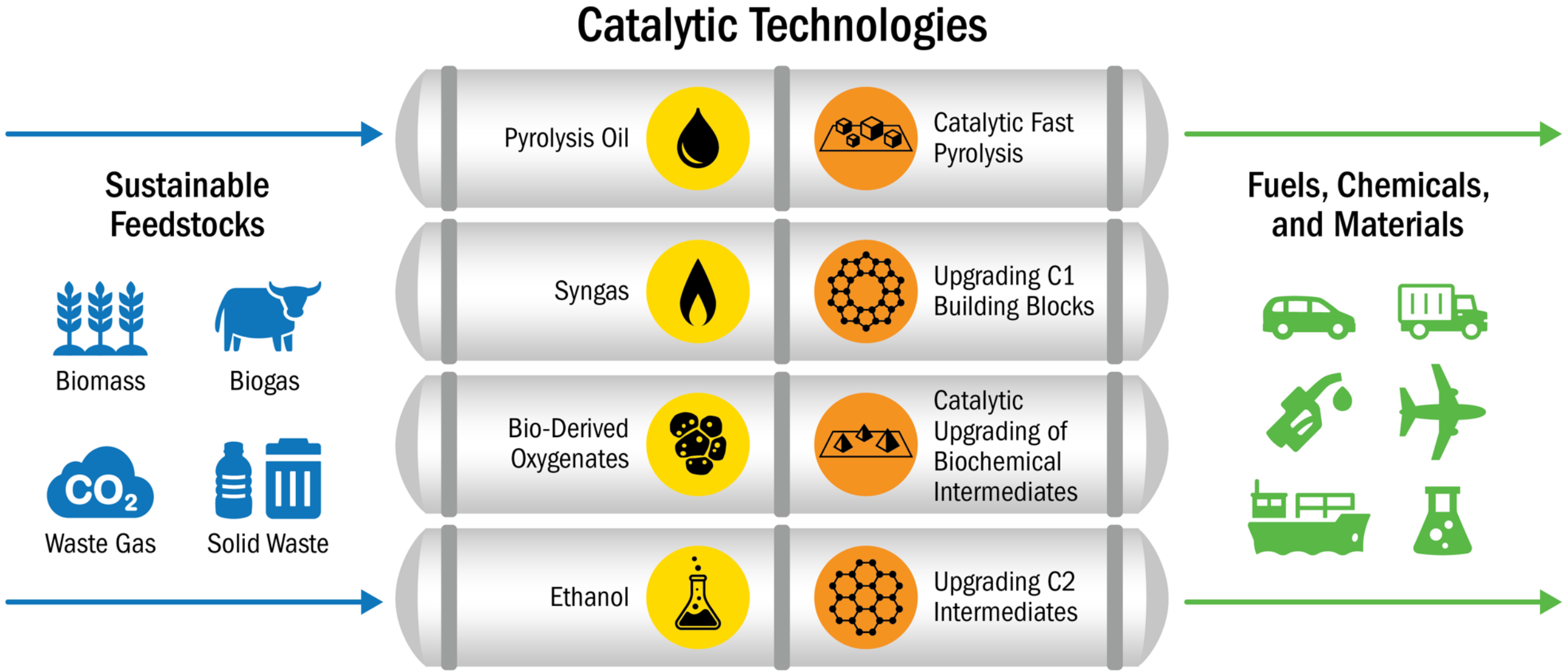
Catalyst Testing





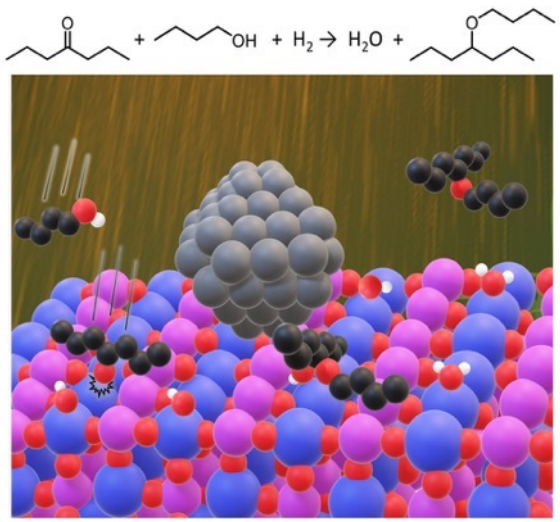
Catalyst Scaling & Process Models

Approach: Pathways Under Development in ChemCatBio



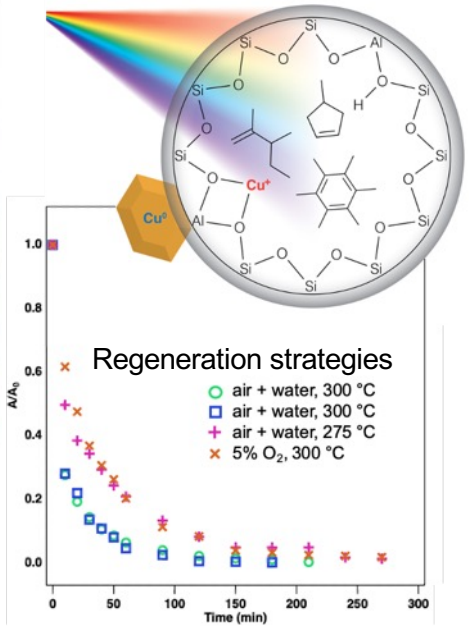
Exploring conversion of multiple feedstocks through multiple processes, targeting SAF as the primary product

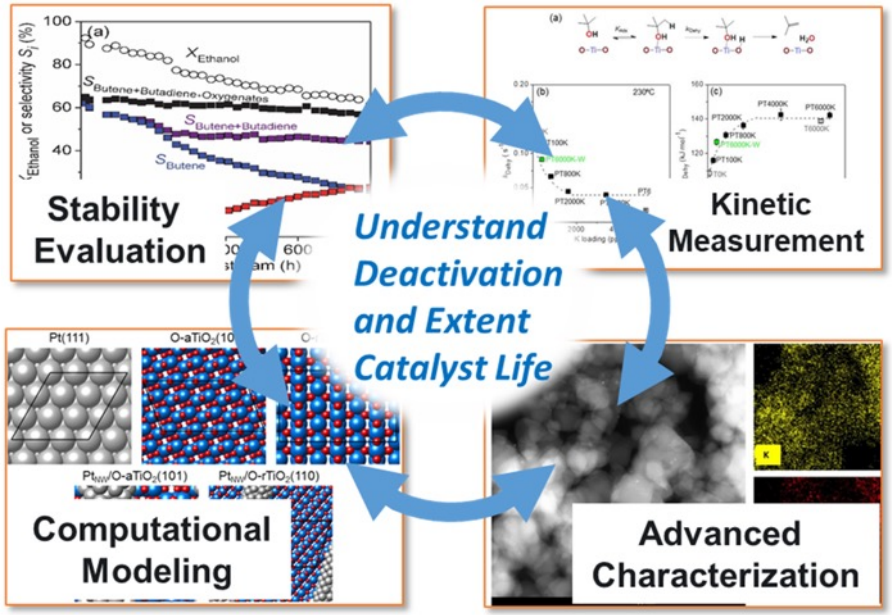
Approach: Enabling Capabilities



Computation

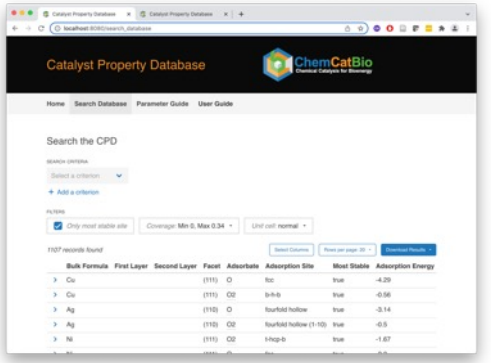
Synthesis & Characterization





Deactivation and Mitigation

Property Database



The Catalyst Property Database

cpd.chemcatbio.org

– Cross-cutting projects that **develop computational tools and experimental methods** to support catalyst and process R&D in ChemCatBio's pathway-specific projects

Key Accomplishments From Prior 2 Years in ChemCatBio

R&D focus on improved yields (i.e., carbon efficiency) for cost reductions

Establishing ChemCatBio as a central hub of knowledge for the bioenergy community

ChemCatBio Team & Impact

Funded by BETO across 8 DOE national labs, we work to connect scientific discovery with market impact

WHO WE ARE

>130
researchers

8
DOE National Labs

BETO
-sponsored

14
Industry Advisory Board Members

OUR IMPACT

SCIENTIFIC CONTRIBUTIONS

>158
publications

42
h-index since 2016

>5,300
citations

1
R&D100 Special Recognition

MARKET IMPACT

3
technology licenses

6
software inventions

29
issued patents and patent applications

12
awarded projects with industry

COMMUNITY RESOURCES

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

11 webinars

2 technology briefs

Directed Funding Opportunities for industry

DEIA Lead Team

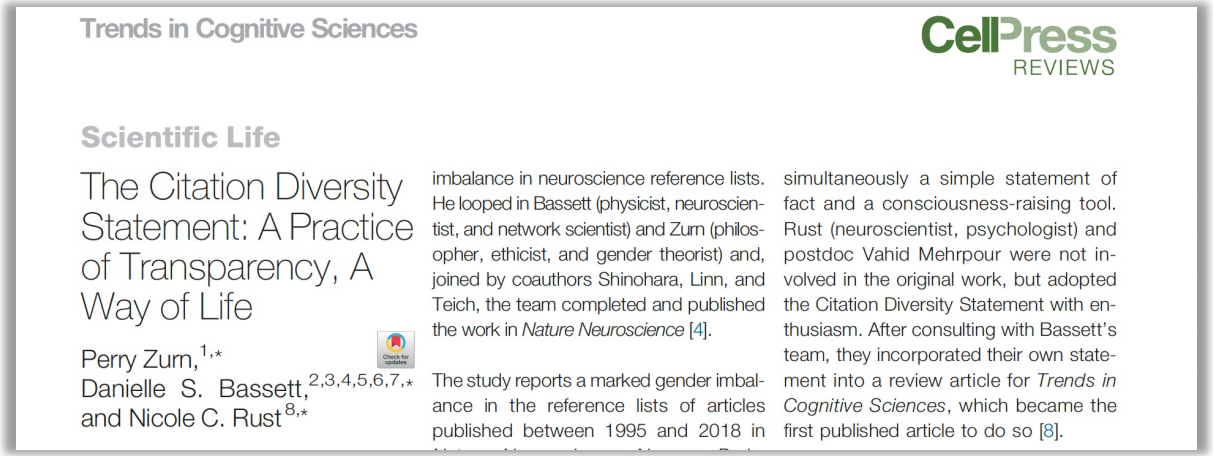
- Established a DEIA Lead Team
- Developed a robust DEIA plan for FY23 – FY25
- FY23: Resources, Training, and Outreach
  - DEIA Resource Library
  - DEI Training
  - Mentorship
  - DEIA Minutes
  - Reciprocal seminars with MSI's
- *FY24 – FY25*: Expanding Impact and Incorporating Energy and Environmental Justice

Anne Starace
(NREL)

Michael Cordon
(ORNL)

Mariefel Olarte
(PNNL)

Example of DEIA Minute: Citation Bias



Trends in Cognitive Sciences

CellPress REVIEWS

Scientific Life

The Citation Diversity Statement: A Practice of Transparency, A Way of Life

Perry Zurn,[1,*] Danielle S. Bassett,[2,3,4,5,6,7,*] and Nicole C. Rust[8,*]

imbalance in neuroscience reference lists. He looped in Bassett (physicist, neuroscientist, and network scientist) and Zurn (philosopher, ethicist, and gender theorist) and, joined by coauthors Shinohara, Linn, and Teich, the team completed and published the work in *Nature Neuroscience* [4].

The study reports a marked gender imbalance in the reference lists of articles published between 1995 and 2018 in

simultaneously a simple statement of fact and a consciousness-raising tool. Rust (neuroscientist, psychologist) and postdoc Vahid Mehrpour were not involved in the original work, but adopted the Citation Diversity Statement with enthusiasm. After consulting with Bassett's team, they incorporated their own statement into a review article for *Trends in Cognitive Sciences*, which became the first published article to do so [8].

Zern et al., *Trends in Cognitive Sciences*, 2020

Community Engagement

- Distributed our **bi-annual newsletter**, *The Accelerator*
- Member of the organizing committee for a series of workshops on **rigor and reproducibility in heterogeneous catalysis**
  - Will result in best practices and guidelines for the community
- Expanded the utility of the **Catalyst Property Database** and published a manuscript in *Nature Catalysis* on **CatCost™** tool
- Established the **ACS CATL – ChemCatBio Graduate Student Travel Award**

Technology Briefs and Newsletter

- **News and recent research reports**
- **Catalysts of Change: Outstanding Early Career Researchers**
  - Highlighting interns, post-docs, and early career researchers within the consortium

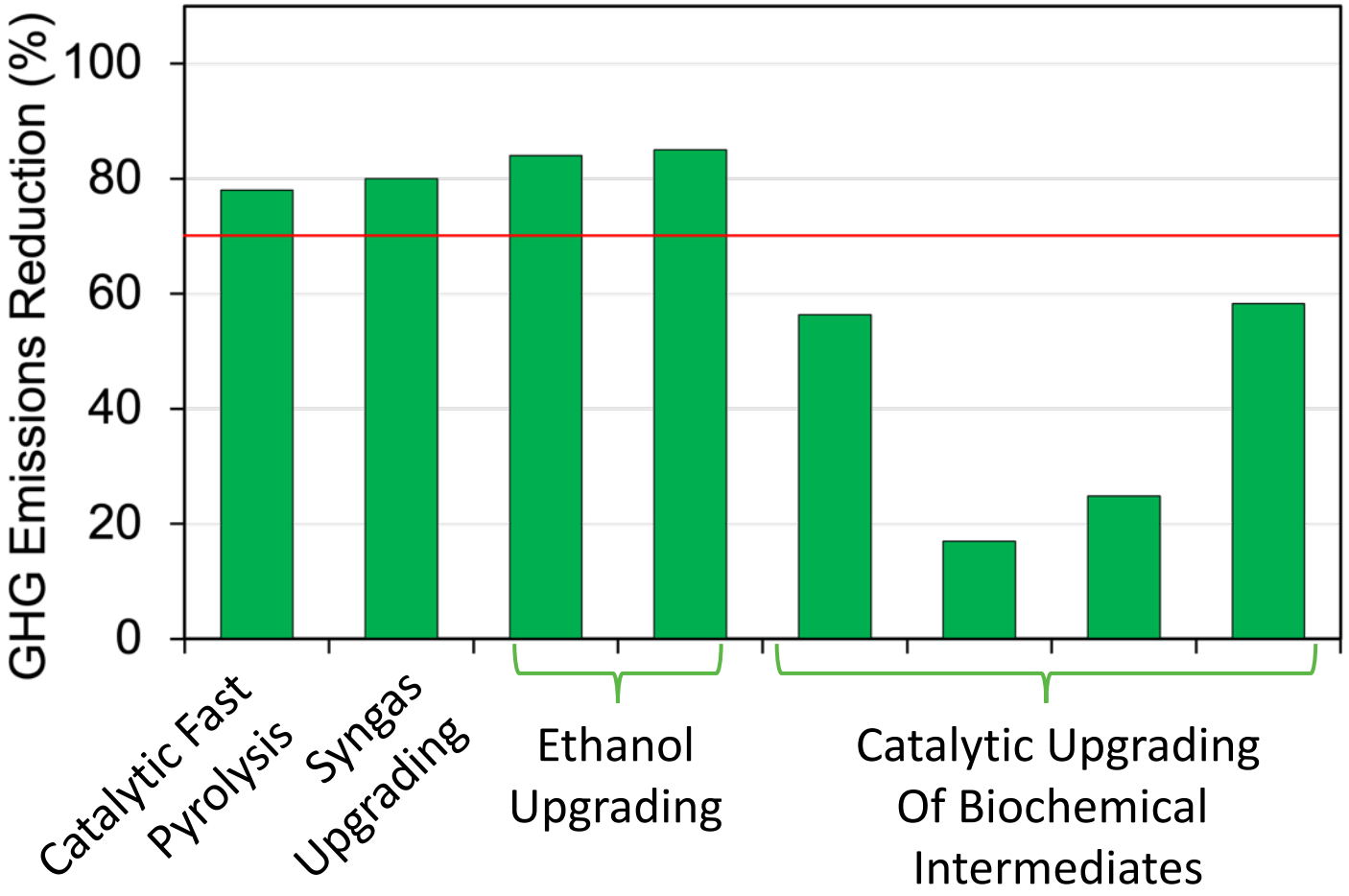
https://www.chemcatbio.org/technology-briefs.html

- **Technology Briefs** provide easy to access reports on emerging catalytic technologies
  - High-level findings from recent publications
  - Risks, challenges, and next steps

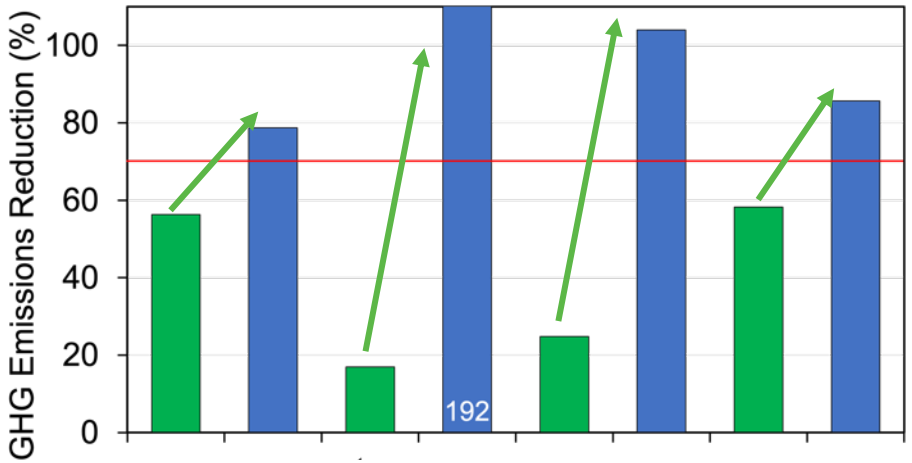
https://www.chemcatbio.org/news-archive.html

Pathway GHG Emissions Reduction

- Multiple pathways exhibit modeled > 70% GHG emissions reduction vs petroleum baseline
- CUBI projects identified future routes to achieve > 70% (e.g., renewable H_2)

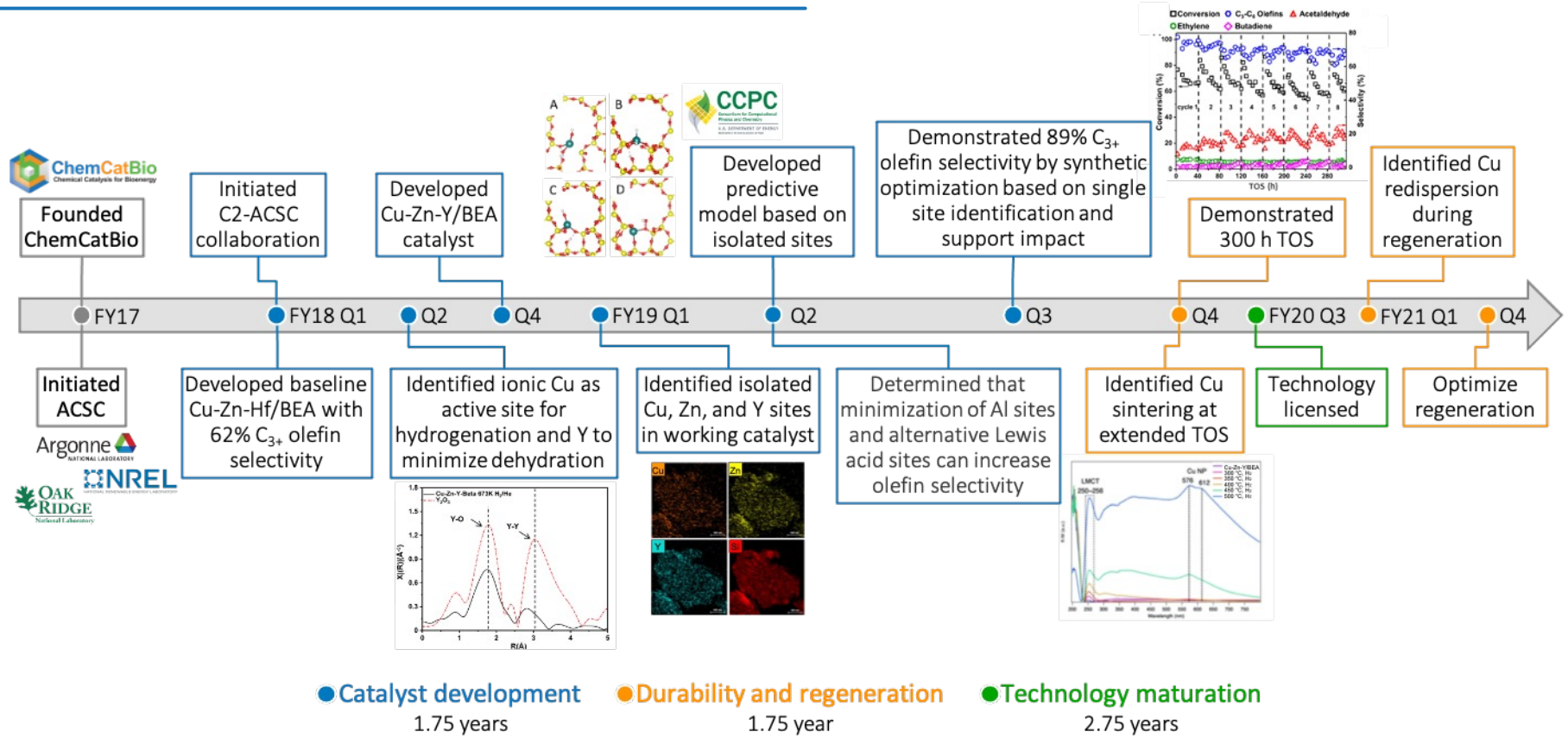


70% reduction



Potential reductions from pathways in Catalytic Upgrading of Biochemical Intermediates project

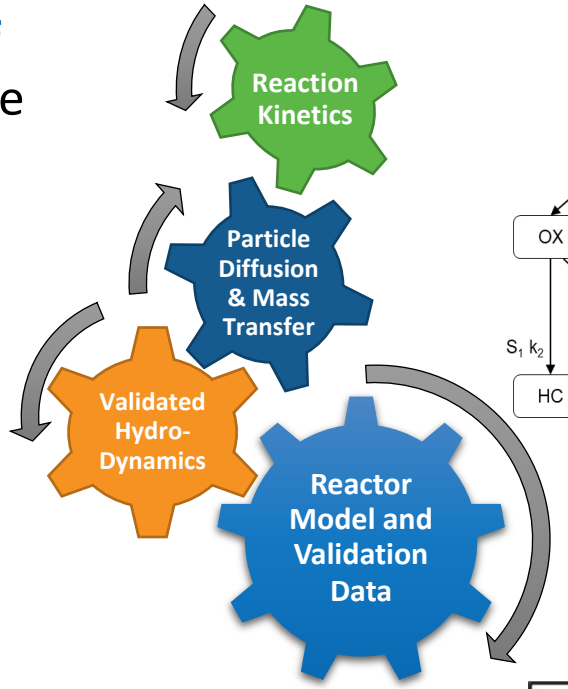
Acceleration of Catalyst and Process Development Cycle

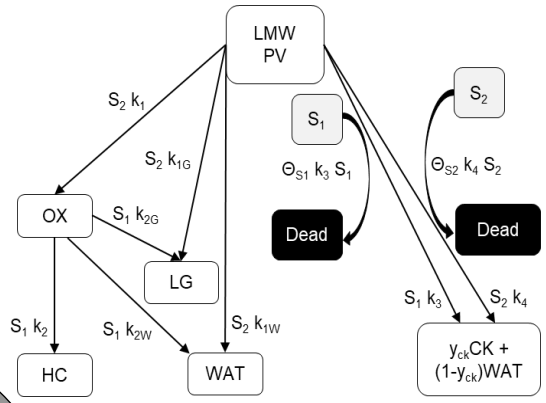


- **Demonstrated a 4x reduction in time** for the **development of a next-gen catalyst** with substantial increase in performance
- In this example, improved C_{3+} olefin selectivity from ethanol was achieved through targeted catalyst design leveraging the **collaborative resources of ChemCatBio**

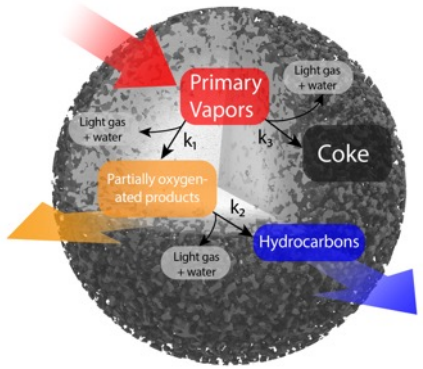
Bioenergy Catalysis Kinetics and Application for Scaleup

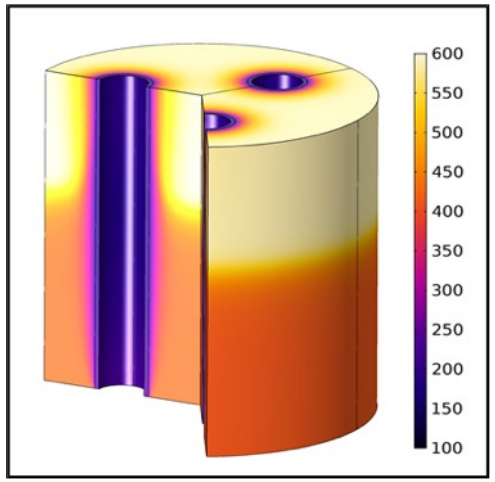
- **Developed a methodology for accurate determination of bioenergy-specific kinetics** and applied kinetics in multiple reactor scale-up models
- Key outcomes:
  - Multicomponent Effectiveness Vector – a new mathematical tool for **analyzing diffusion limitations for cascade reaction mechanisms** in catalyst pellets
  - **Kinetics** in both fluidized bed (computational fluid dynamic model) and fixed bed models
  - Validated methodology and kinetics **at multiple scales**
- Impact:
  - **Predictive** guidance for key decision making in Catalytic Fast Pyrolysis Verification
  - Applied capabilities **to enable scale-up** of bioenergy processes for Pyran and Catalyxx





CCPC
Consortium for Computational Physics and Chemistry
U.S. DEPARTMENT OF ENERGY
BIOENERGY TECHNOLOGIES OFFICE





Pyran Catalyxx

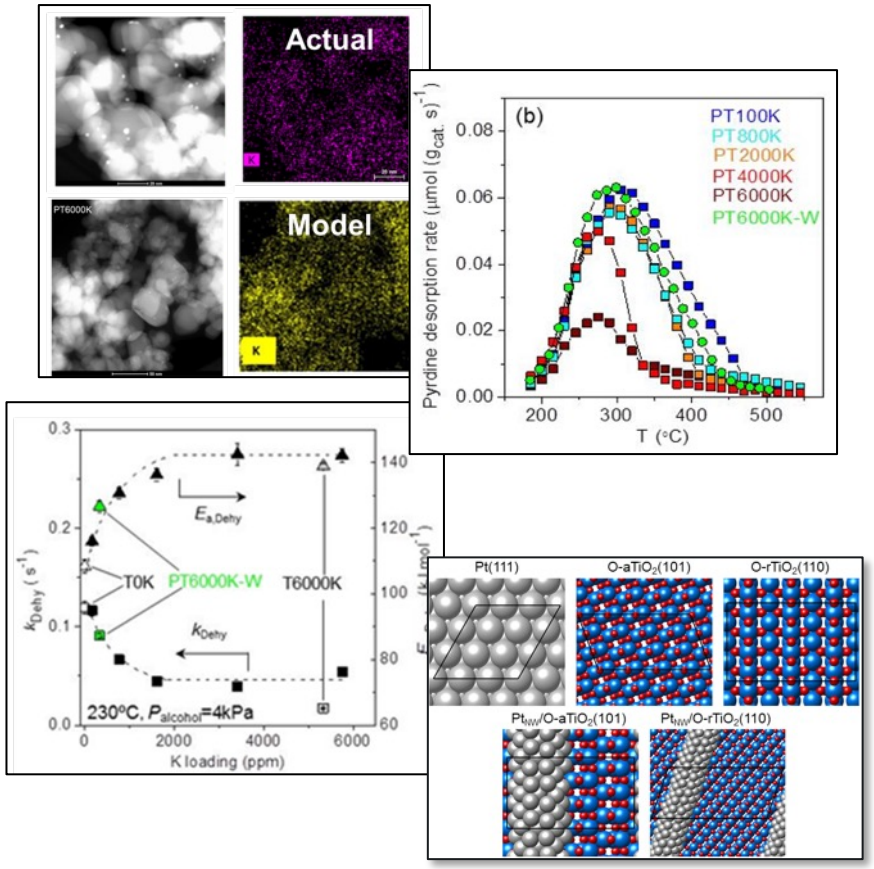
https://www.energy.gov/eere/bioenergy/beto-webinars

Addressing Overarching Catalyst Deactivation Challenges

- ChemCatBio teams work collaboratively and coordinately to improve catalyst lifetime and address overarching catalyst deactivation challenges

- Developed a comprehensive understanding of the impact of inorganics (K) on different types of active sites on typical multifunction catalysts
  - *ACS Catalysis* **2022**, *12*, 465-480
  - *ACS Catalysis* **2022**, *12*, 13555-13599

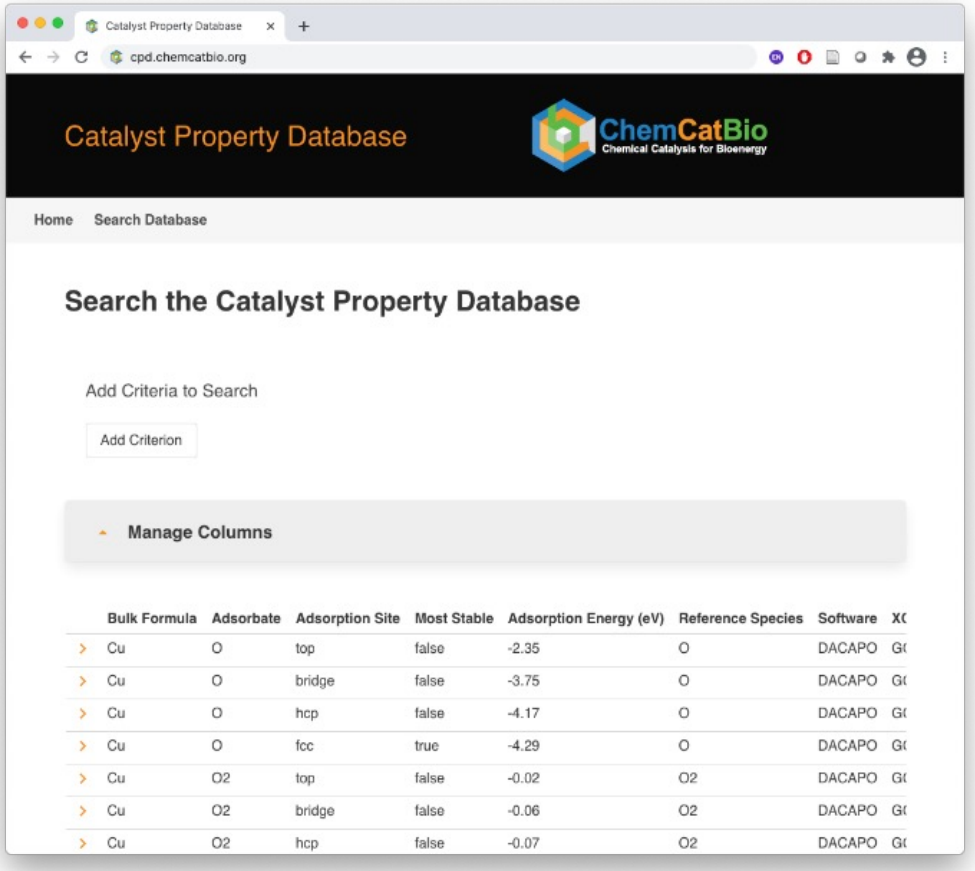
Established structure-performance relationship and precise description of the atomic-level interaction of K^+ with catalyst active sites



Sets the basis for continued R&D through FY25 to mitigate the risk of catalyst deactivation in our processes

Catalyst Property Database

- The Catalyst Property Database (CPD) is designed to accelerate catalysis R&D with a centralized, searchable repository of catalyst properties
- **Publicly released in Sept 2020** and currently houses theoretically computed, published (i.e., peer-reviewed) adsorption energies for reaction intermediates on catalytic surfaces
- In fall of 2021, the CPD opened for **community data addition**



A public webinar on CPD can be found on our website: www.chemcatbio.org

cpd.chemcatbio.org

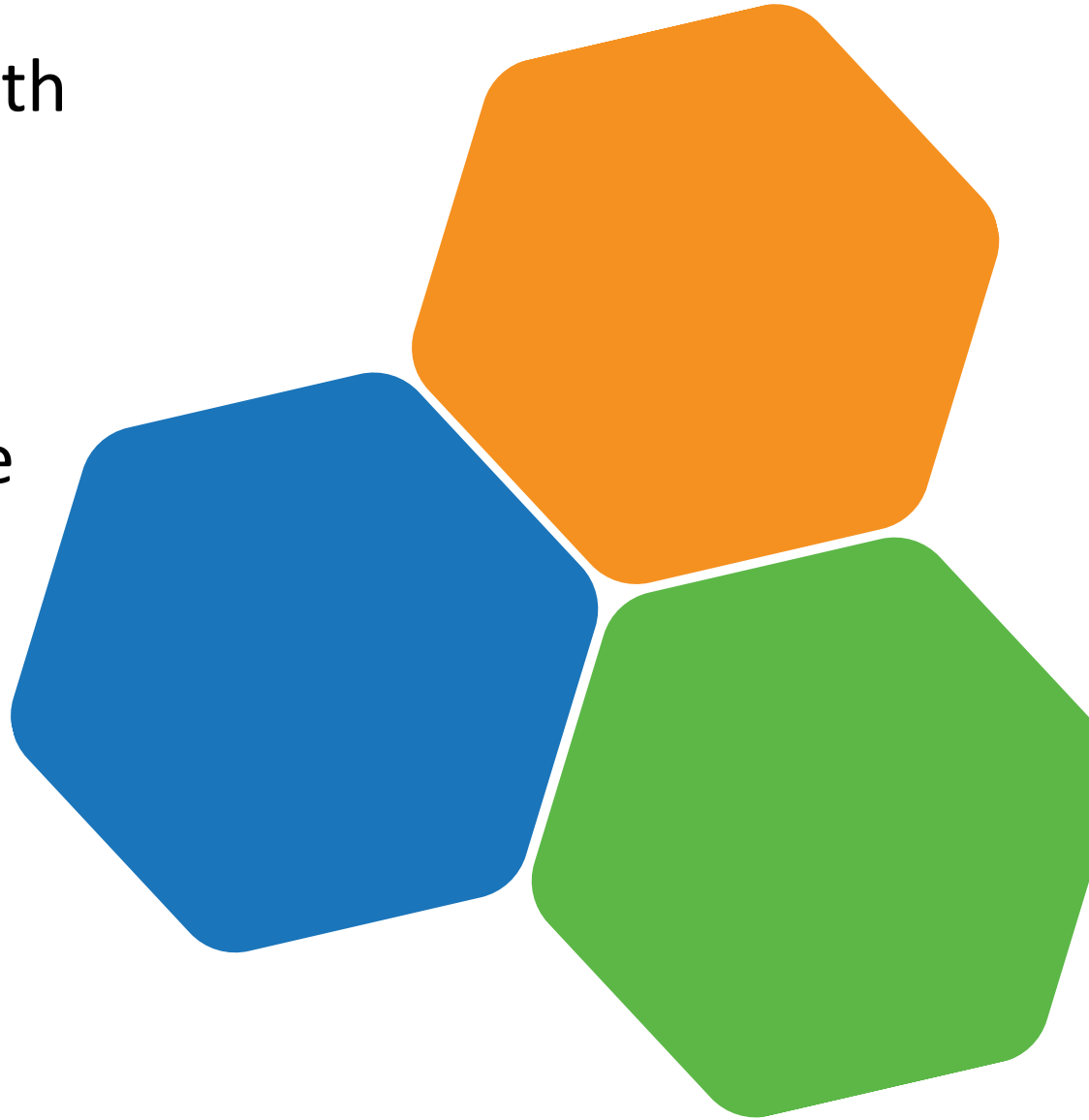
Free and public R&D resource

Consortium Goals for 2023-25

2023-25 Focus Areas

Process integration and fuel production with engineered catalysts to enhance industrial partnerships.

ChemCatBio as a central hub of knowledge for the bioenergy community.

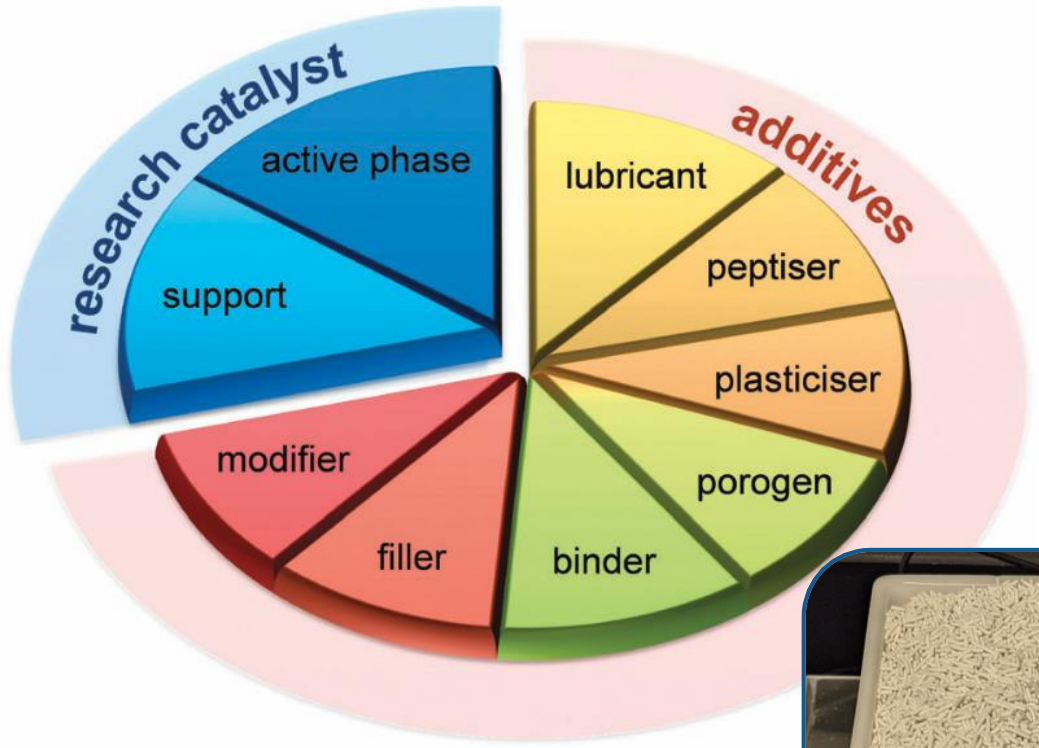


FY25 End-of-Project Milestone: Develop and advance biomass and waste conversion technologies for hard-to-decarbonize fuels and chemicals, and provide foundational knowledge to address risks associated with catalyst/process durability and carbon efficiency.

Advancing and Derisking Technologies Using Engineered Catalysts

How can we bridge the gap between lab-scale powders and pilot-scale formed catalysts?

What is an “Engineered” Catalyst?



An engineered or technical catalyst is a multicomponent catalyst formulation that possesses additives and structural components required for operation in a commercial reactor

- Physical: mass/heat transfer
- Chemical: functionality
- Mechanical: strength, attrition resistance

Mitchell et al., *Chem. Soc. Rev.,* 2013, 42, 6094.

Approach to Working With Engineered Catalysts

- **Option 1**

Evaluate **off-the-shelf, commercial materials** from industrial partners

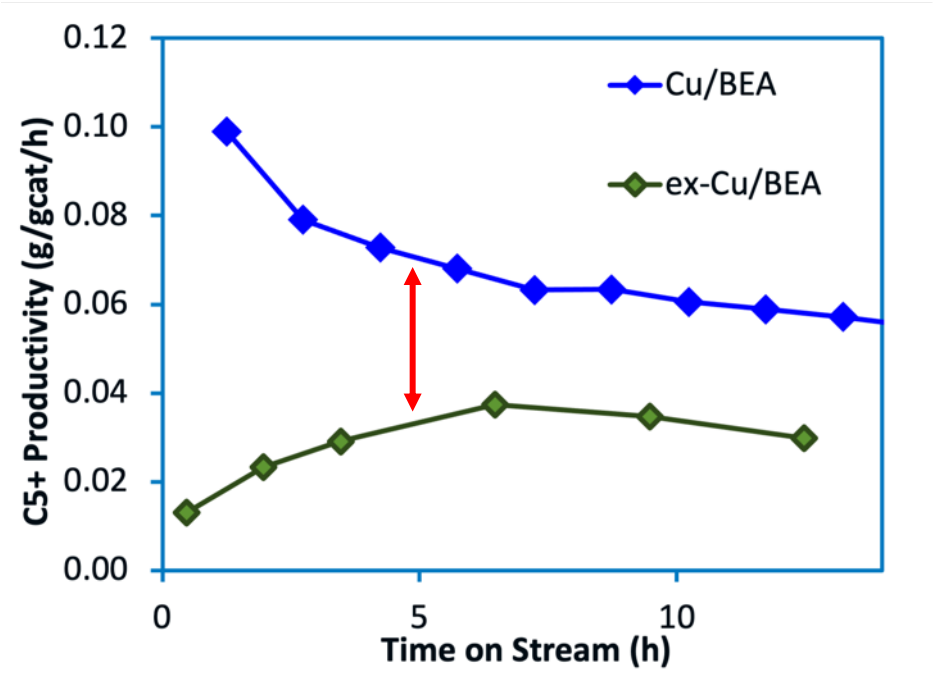
- **Option 2**

Work with industrial partners who can **prepare engineered formulations and iterate performance testing** to develop a commercial-ready material

- **Option 3**

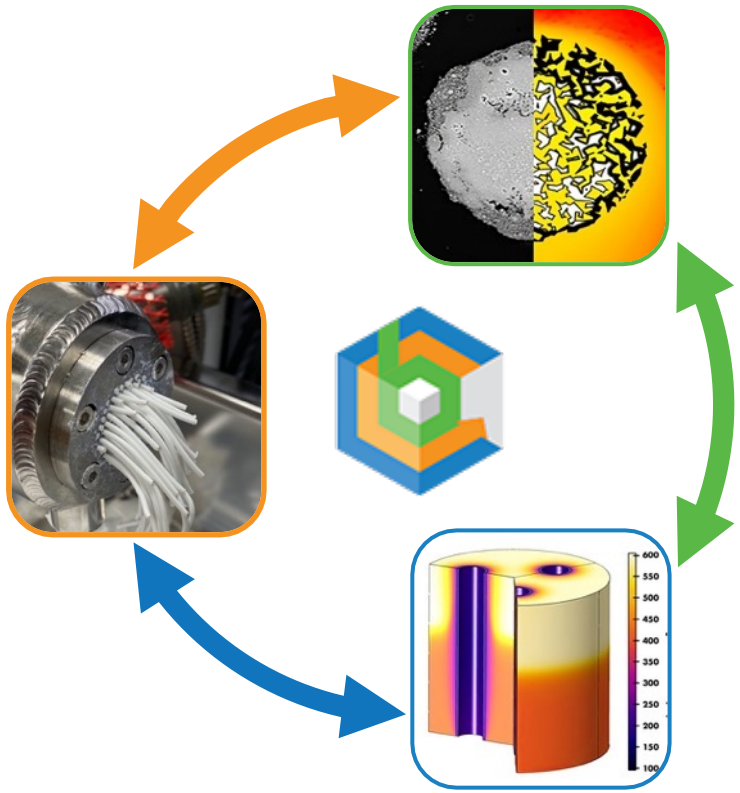
For **pre-commercial catalysts**, develop the **in-house capability** to determine the **structure-property-performance relationships** that inform the transition to engineered forms

- *Transition of Cu/BEA catalyst (syngas project) for 2018 pilot project was **non-trivial***
  - Lower than desired activity observed
  - Identified the need to answer specific questions to advance technology with engineered catalysts



Engineered Catalyst Forms (Option 3)

Objective: Enable CCB pathway technologies to **evaluate the catalytic performance of realistic** engineered catalysts and **develop structure-property relationships** with engineered forms



- Addresses the **non-trivial transition** from research to engineered catalysts forms
  - Challenge in maintaining highly-tailored catalyst functionalities
- **Reduces the risk of commercialization** by reducing uncertainty in engineered catalyst operability
  - Loss of activity/selectivity/lifetime due to binder, porosity, and/or change in active site structure

Year 1 Goal – Determine impact of engineered catalyst formulation on **Cu speciation and deactivation in Cu/BEA catalyst**, and correlate with performance.

Industry Engagement

ChemCatBio has **demonstrated industry engagement across catalytic technologies** and will build new partnerships towards commercialization

Types of Partnerships With ChemCatBio

Industry Advisory Board (IAB)

- Volunteers advise ChemCatBio strategy for work to be industry-relevant
  - Consortium-level and project-level advisory boards
- Representatives from fuels & chemicals industry, large industrial & start-ups

Co-Operative Research and Development Agreement (CRADA)

- Funds-in from partner to ChemCatBio to perform R&D on a specific ChemCatBio technology

Direct Funding Opportunity (DFO)

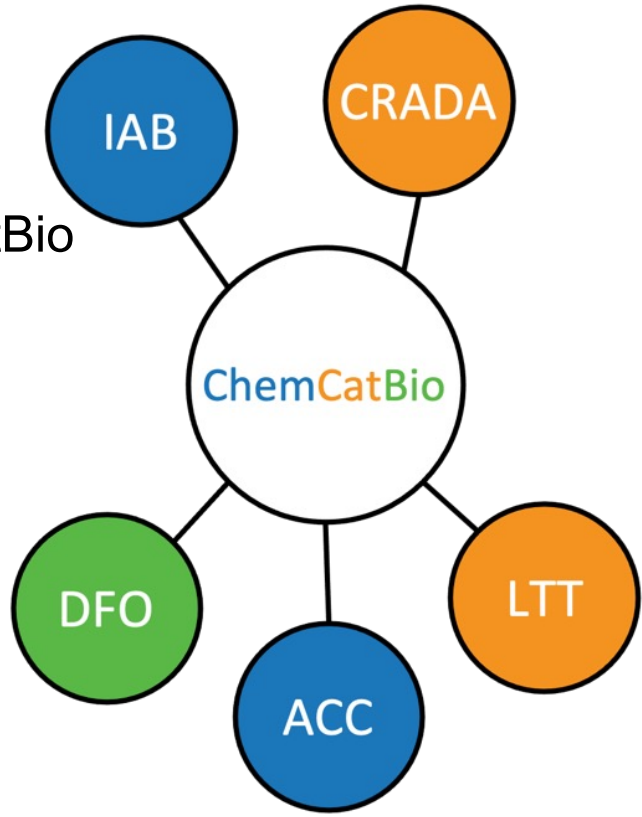
- Funds from BETO to generate a new ChemCatBio project based on a joint proposal between industry and ChemCatBio researchers to solve a specific industry problem

Licensing/Technology Transfer (LTT)

- External development/commercialization of a ChemCatBio technology (no ChemCatBio participation required)

Accelerator Partnership (ACC)

- Strategic consortium-level partnership to support Enabling Capabilities, not specific pathways/technologies
- No funds change hands, goal to develop joint value for ChemCatBio and partner



Accelerator Partnerships

Strategic consortium-level partnership to support ChemCatBio enabling capabilities

- Core ChemCatBio enabling capabilities:
  - Catalyst characterization
  - Computational modeling
  - Catalyst evaluation and benchmarking
- Work side-by-side with industry to advance capabilities in these areas needed to support bioenergy technologies

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Inspiring science, enhancing life

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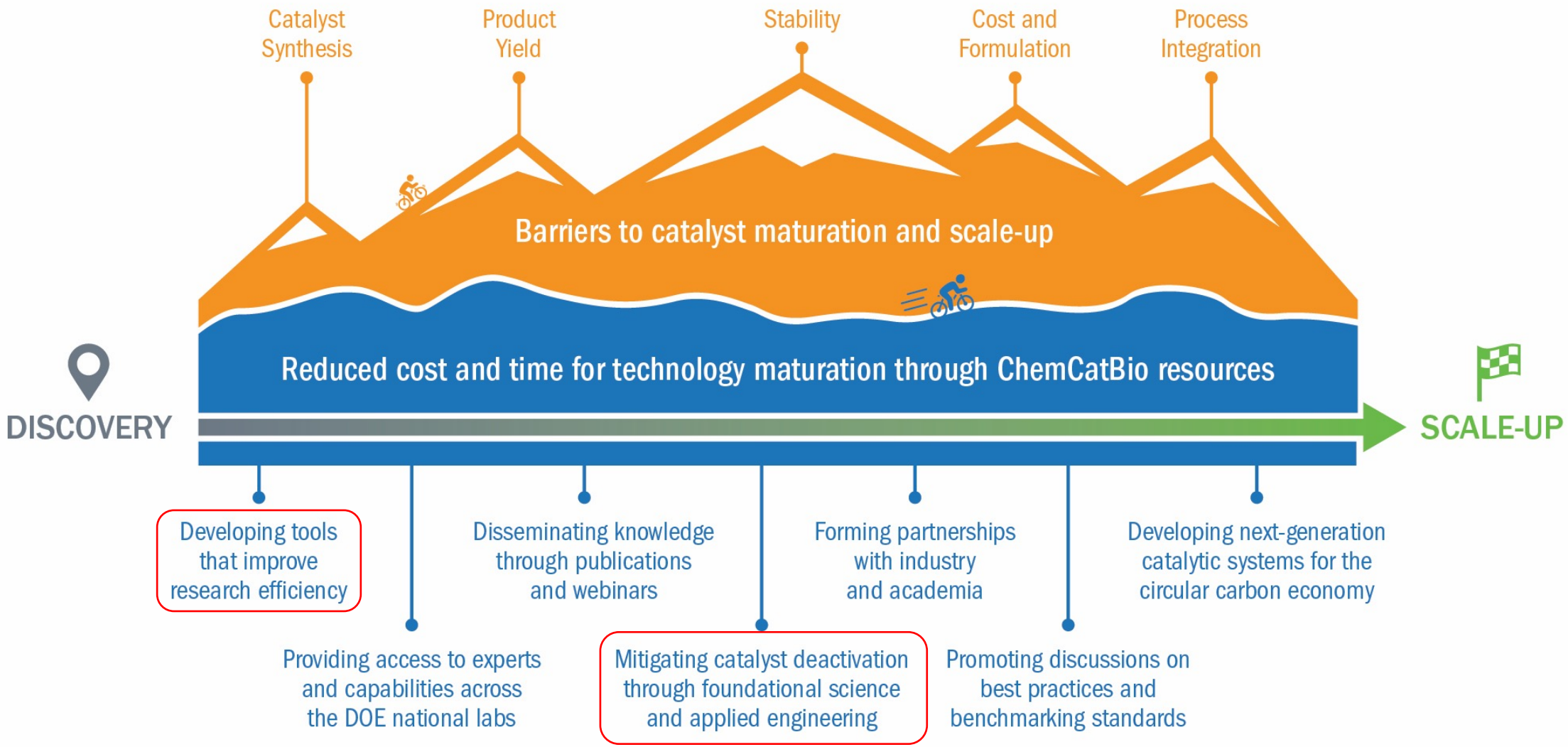
IBM

Accelerating Catalyst Design

Central Hub of Knowledge

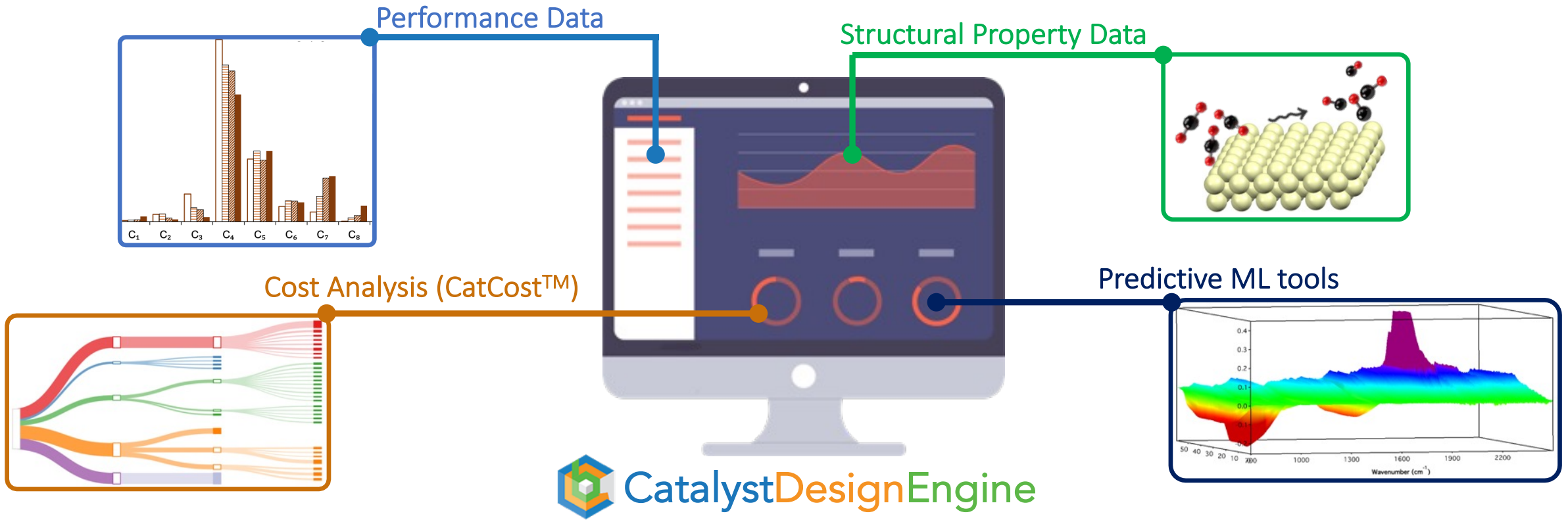
The path to catalyst deployment is slow and difficult.



ChemCatBio is accelerating the catalyst and process development cycle.

Catalyst Design Engine: Vision

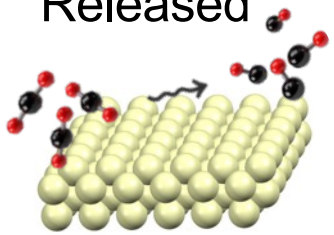
To support and accelerate catalysis RD&D by addressing barriers with a suite of predictive analytical tools



Integrating database technology from **Datahub** with cost estimation from **CatCost** at the **frontier of machine learning** to transform catalyst design and deployment

Catalyst Design Engine: Progress and Goals

Surface Phase Explorer Released



Public Release of CatCost

Public Release of CPD

Release Catalyst Deactivation Mitigation Dataset in CPD

Collaboration on Machine Learning in CPD

Release the First Public CDE Demonstration on Catalyst Deactivation Mitigation

FY15 16 18 19 20 21 22 23 25

CatCost Funded in ChemCatBio

Tested a Proof-of-Concept CDE Implementation

CPD open to External Uploads

Release CDE Predictive Capabilities for Specific CCE Core Technologies

Summary

- Catalysis is essential for decarbonization and to meet the SAF Grand Challenge
- Biomass as a feedstock introduces unique challenges that must have dedicated R&D
- ChemCatBio seeks to accelerate the catalyst and process development cycle to help shorten the time to market for renewable technologies
  - Process integration and fuel production with engineered catalysts to enhance industrial partnerships
  - A central hub of knowledge for the bioenergy community

Acknowledgements

Dan.Ruddy@nrel.gov

- CCB Director: Josh Schaidle
- Bioenergy Technologies Office: Kevin Craig, Sonia Hammache, Trevor Smith, Ian Rowe
- Industry Advisory Board Members and Collaborators
- CCB Steering Committee

Rajeev Assary	Fred Baddour	Robert Dagle	Vanessa Dagle	Carrie Farberow
Jack Ferrell	Mike Griffin	Susan Habas	David Johnson	Ted Krause
Jeffrey Linger	Mariefel Olarte	Karthi Ramasamy	Jim Parks	Asanga Padmaperuma
Andrew Sutton	Kinga Unocic	Huamin Wang	Claire Yang	

ChemCatBio
Chemical Catalysis for Bioenergy

Energy Materials Network
U.S. Department of Energy

This work was performed in collaboration with the Chemical Catalysis for Bioenergy Consortium (ChemCatBio, CCB), a member of the Energy Materials Network (EMN)

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

Acknowledgements

NREL
NATIONAL RENEWABLE ENERGY LABORATORY
Argonne NATIONAL LABORATORY
Pacific Northwest NATIONAL LABORATORY
Sandia National Laboratories
OAK RIDGE National Laboratory
INL Idaho National Laboratory
Los Alamos NATIONAL LABORATORY EST. 1943
NATIONAL ENERGY TECHNOLOGY LABORATORY

Quad Chart Overview

Timeline
- *10/01/2022*
- *09/30/2025*

	FY22 Costed	Total Award
DOE Funding	*$220k*	*$230k for FY23* *$690k for FY23-25*

TRL at Project Start: *2*
TRL at Project End: *2*

Project Goal

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

End of Project Milestone

Develop and advance biomass and waste conversion technologies for hard-to-decarbonize fuels and chemicals, and provide foundational knowledge to address risks associated with catalyst/process durability and carbon efficiency fuel property analysis.

Funding Mechanism

AOP LabCall 2023 - ChemCatBio

Project Partners*
- N/A

Responses to Previous Reviewers' Comments

- **Comment:** ChemCatBio provides a unique platform that enables researchers to accelerate the development of catalysts and relevant technologies for bioenergy applications. This unique platform gathers researchers with a wide variety of backgrounds and expertise, creating the opportunity for interdisciplinary research. It would be beneficial to create a mechanism that makes everyone's voice heard, especially for such a large group of researchers. It could also benefit if we could use tools such as Teams and Zoom that could enable "virtual" meetings and discussion. Such tools may change the way we do research even after the pandemic. The research of ChemCatBio shows significant advancement in the last 2 years and is on its path toward the DOE BETO goal of affordable bio-based fuel. This research would fundamentally impact society. It could be beneficial if the research could leverage more power of artificial intelligence, computation, and advanced characteristics. Indeed, some technologies themselves are still in the early stage, such as machine learning, though they are advancing rapidly. It could be useful if they can be integrated into the research of ChemCatBio more closely.

  - Response: Building on our progress to date, we will use the reviewers' feedback to guide our work in the coming years, especially in the areas of (1) defining KPIs/metrics for the consortium, (2) enabling the technology transition toward scale-up and integration within the BETO program, (3) developing and leveraging tools (e.g., artificial intelligence, high-throughput synthesis/testing, and durability testing rigs) that facilitate further acceleration of the catalyst and process development cycle, (4) supporting effective collaboration and communication mechanisms that enable every person within the consortium to have a voice and to be heard, and (5) expanding and extending catalyst durability tests to accurately identify deactivation mechanisms that may plague commercial operation.

Publications, Patents, Presentations, Awards, and Commercialization

- Publications since Peer Review in 2021
  - N/A
- Presentations since Peer Review in 2021
  1. “Using Chemistry and Engineering to Accelerate Technology Development for Sustainable Transportation Fuels” invited seminar at Lafayette College, Easton, PA, Nov 18, 2022.
  2. “The Next Three Years of Catalyst R&D To Decarbonize Fuels and Chemicals” ChemCatBio Webinar Series, Dec 14, 2022.
  3. "What's Next for ChemCatBio", Invited Presentation, ABLC Next 2022, San Francisco, CA, October 27th, 2022
  4. "Accelerating the Catalyst and Process Development Cycle for Bioenergy Applications", ACS National Meeting, August 23rd, 2022
  5. "Accelerating the Catalyst and Process Development Cycle for Bioenergy Applications", North American Catalysis Society Meeting, New York, New York, May 25th, 2022.
  6. "Accelerating the Catalyst and Process Development Cycle for Bioenergy Applications", Invited Seminar, University of Delaware, April 29th, 2022.
  7. “The Chemical Catalysis for Bioenergy Consortium”, Invited Presentation, Advanced Bioeconomy Leadership Conference 2022, Washington, DC, March 17th, 2022.
  8. “Accelerating the Catalyst and Process Development Cycle for Bioenergy Applications”, Invited Presentation, 240th Electrochemical Society Meeting, October 12th, 2021.
  9. “Catalysis for Bioenergy”, Invited Lecture, Texas A&M University, September 1st, 2021.
- Patents since Peer Review in 2021 (9 total since 2017)
  - N/A
- Commercialization update
  - N/A