Pursuing the rapid decarbonization of our economy

Accelerating the catalyst and process development cycle for bioenergy applications

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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)

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

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

Photo courtesy of istock.com
https://www.energy.gov/eere/bioenergy/sustainable-aviation-fuel-grand-challenge

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

Computation

Foundational Catalysis Science

Catalyst Testing

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

Applied Engineering

Catalyst Scaling & Process Models
Exploring conversion of multiple feedstocks through multiple processes, targeting SAF as the primary product.
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
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**
- >158 publications
- 42 h-index since 2016
- >5,300 citations
- 1 R&D100 Special Recognition
- 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

Example of DEIA Minute: Citation Bias

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

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 H₂)

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 Catalyx

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

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
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

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
Accelerating Catalyst Design

Central Hub of Knowledge
The path to catalyst deployment is slow and difficult.

Barriers to catalyst maturation and scale-up

Reduced cost and time for technology maturation through ChemCatBio resources

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
- Collaboration on Machine Learning in CPD
- Release Catalyst Deactivation Mitigation Dataset in CPD
- Release the First Public CDE Demonstration on Catalyst Deactivation Mitigation
- Release CDE Predictive Capabilities for Specific CCB Core Technologies

- CatCost Funded in ChemCatBio
- Tested a Proof-of-Concept CDE Implementation

CPD open to External Uploads
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

- **CCB Director**: Josh Schaidle
- **Bioenergy Technologies Office**: Kevin Craig, Sonia Hammache, Trevor Smith, Ian Rowe
- **Industry Advisory Board Members and Collaborators**
- **CCB Steering Committee**
  
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This work was performed in collaboration with the Chemical Catalysis for Bioenergy Consortium (ChemCatBio, CCB), a member of the Energy Materials Network (EMN)
Acknowledgements
## Quad Chart Overview

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

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<th>FY22</th>
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### 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.

### TRL at Project
- TRL at Project Start: 2
- TRL at Project End: 2

### 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**

- **Patents since Peer Review in 2021 (9 total since 2017)**
  - N/A

- **Commercialization update**
  - N/A