ChemCatBio
Chemical Catalysis for Bioenergy

The Next Three Years of Catalyst R&D To Decarbonize Fuels and Chemicals

Daniel Ruddy, Deputy Director

December 14, 2022

Housekeeping

- Attendees will be in listen-only mode
- Audio connection options:
  - Computer audio
  - Dial in through your phone (best connection)
- Automated closed captions are available
- Use the Q&A panel to ask questions
- Technical difficulties? Contact Erik Ringle through the chat section, lower right of your screen
- Recording will be available at: https://www.chemcatbio.org/webinars.html

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Today's Speaker

Dan Ruddy

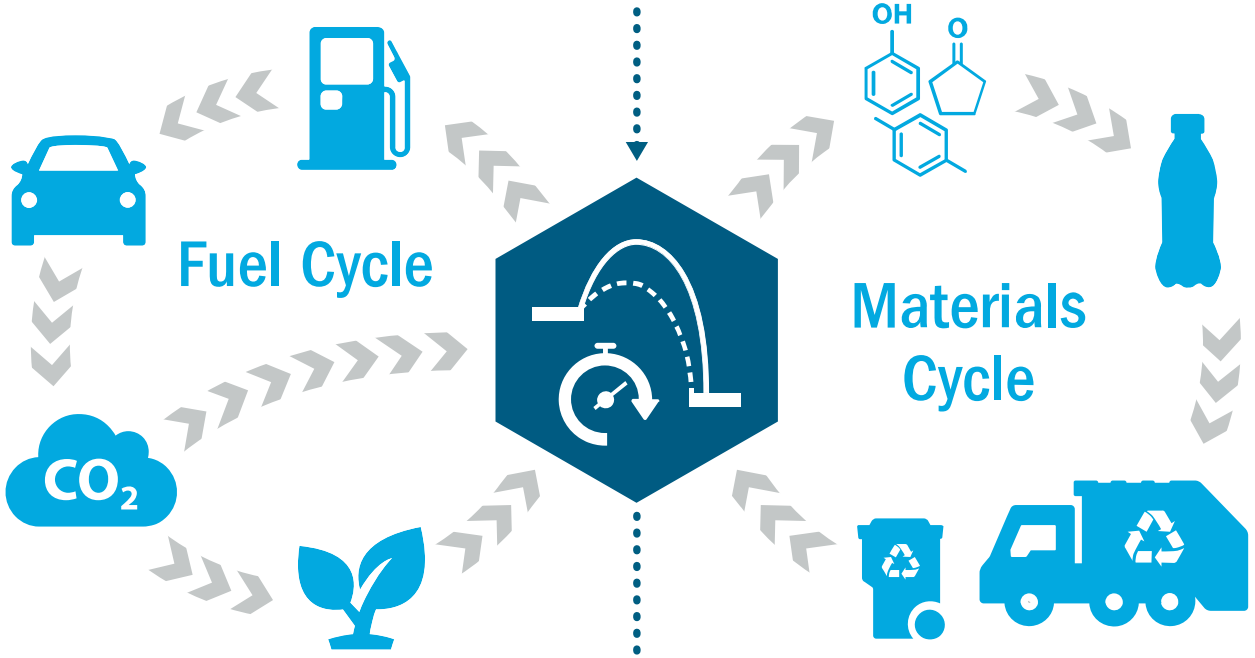
ChemCatBio Deputy Director

Senior Scientist, National Renewable Energy Laboratory

Accelerating Discovery and Development

Catalysis enables a circular carbon economy.

85% of industrial chemical processes rely on catalysts.

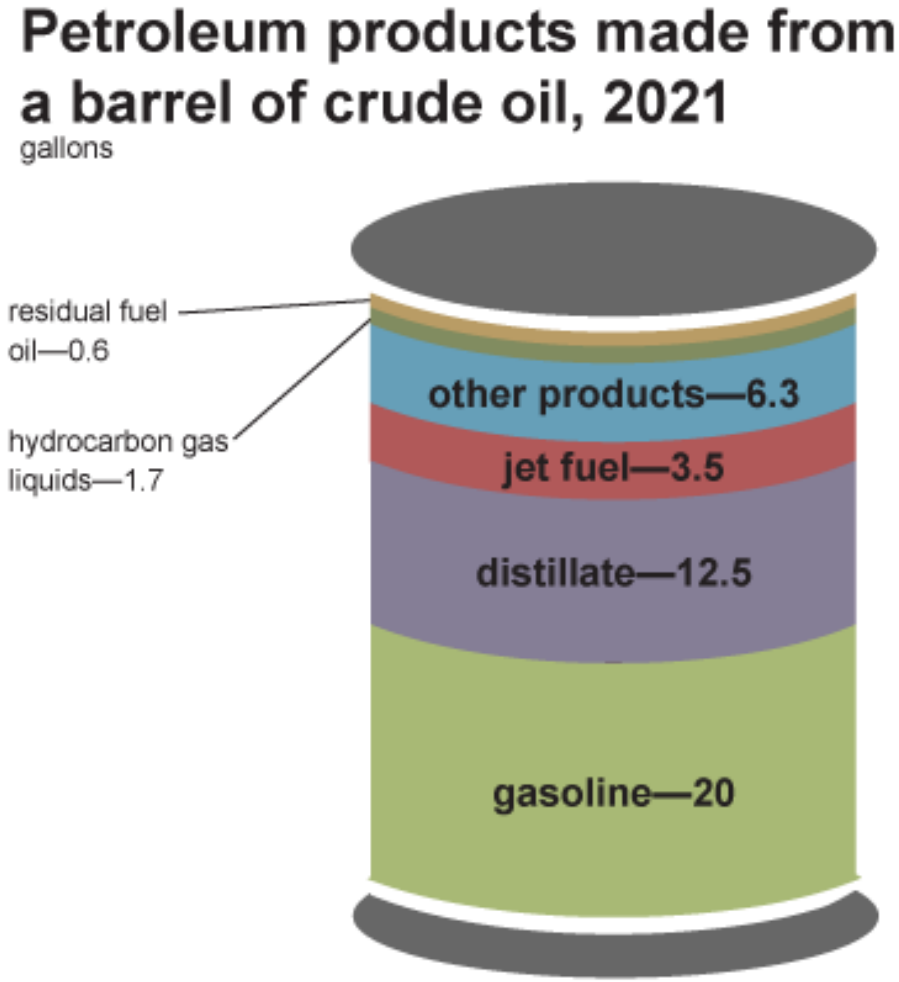


ChemCatBio is accelerating catalyst development for bioenergy applications

The Challenge – Need Tons of Fuel

Transportation Fuel Demand in the US

- 70% of energy used from petroleum is transportation fuel
- 85% of a barrel of oil goes to transportation fuel
- 19.9 Million barrels per day
- 7.3 Billion barrels per year
  - US only, 2021



Source: U.S. Energy Information Administration, *Petroleum Supply Monthly*, March 2022, preliminary data
Note: A 42-gallon (U.S.) barrel of crude oil yields about 45 gallons of petroleum products because of refinery processing gain. The sum of the product amounts in the image may not equal 45 because of independent rounding.

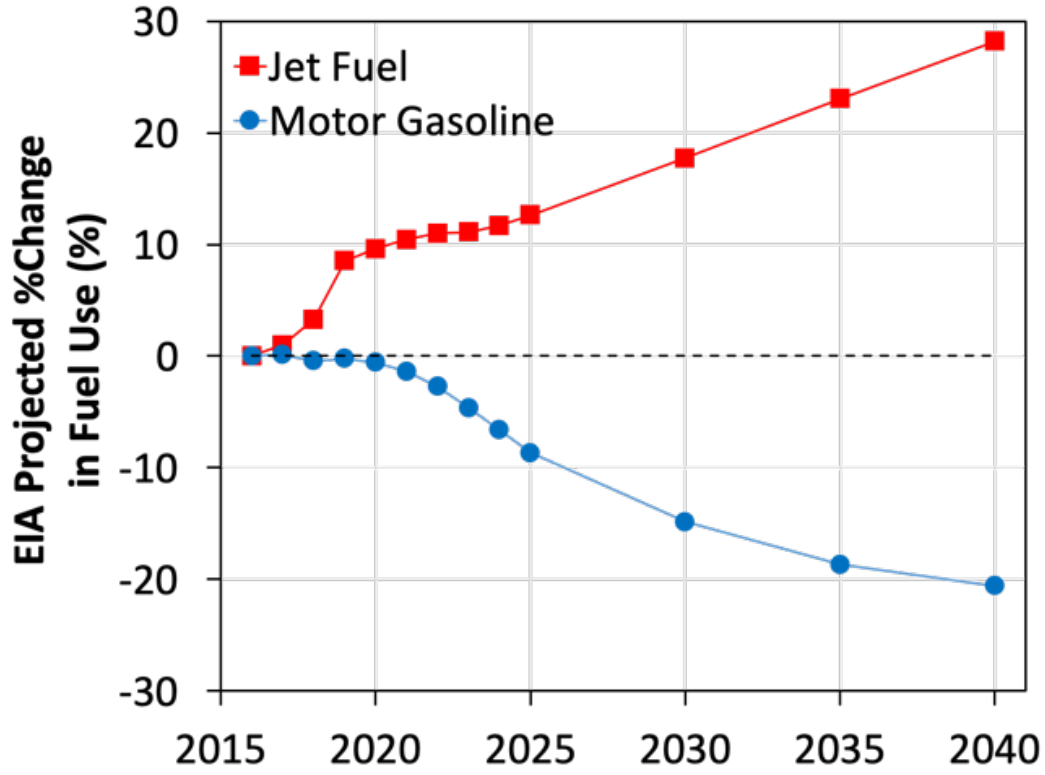
The Challenge – Need Tons of Fuel

Gasoline: 135 billion gallons per year

Diesel: 60 billion gallons per year

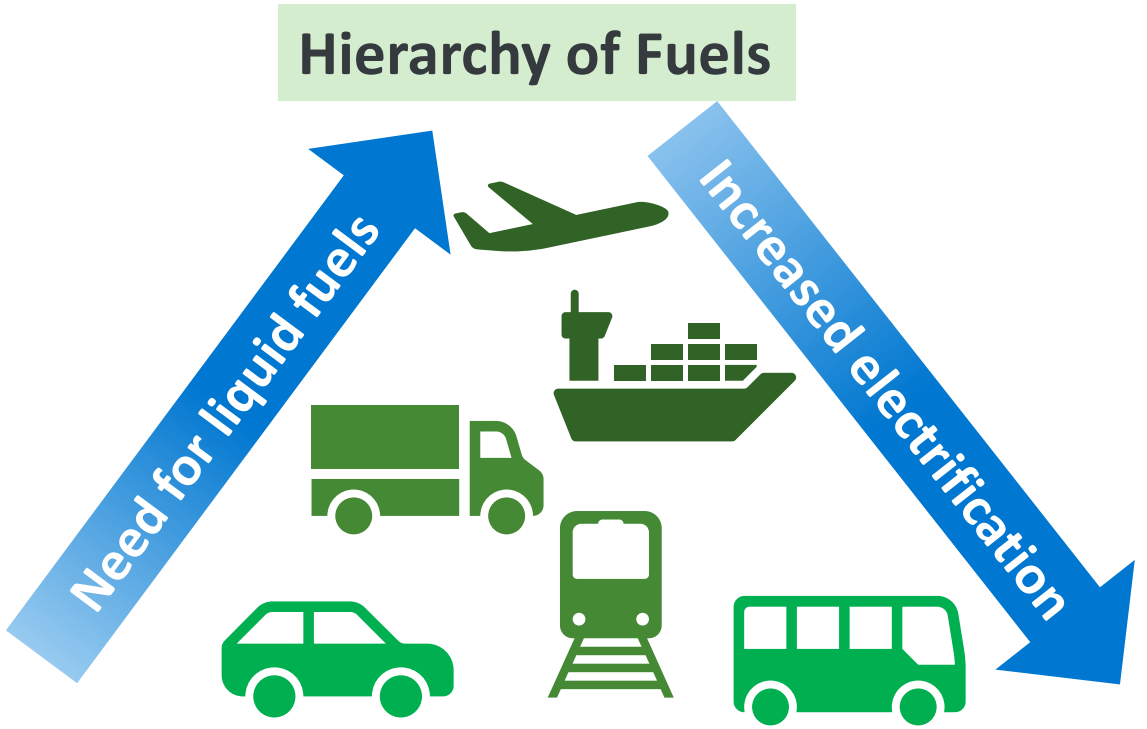
Jet: 21 billion gallons per year

But the needs are changing



Data from U.S. Energy Information Administration

Electrification can displace gasoline, not jet



The Opportunity – Have Tons of Biomass

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

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

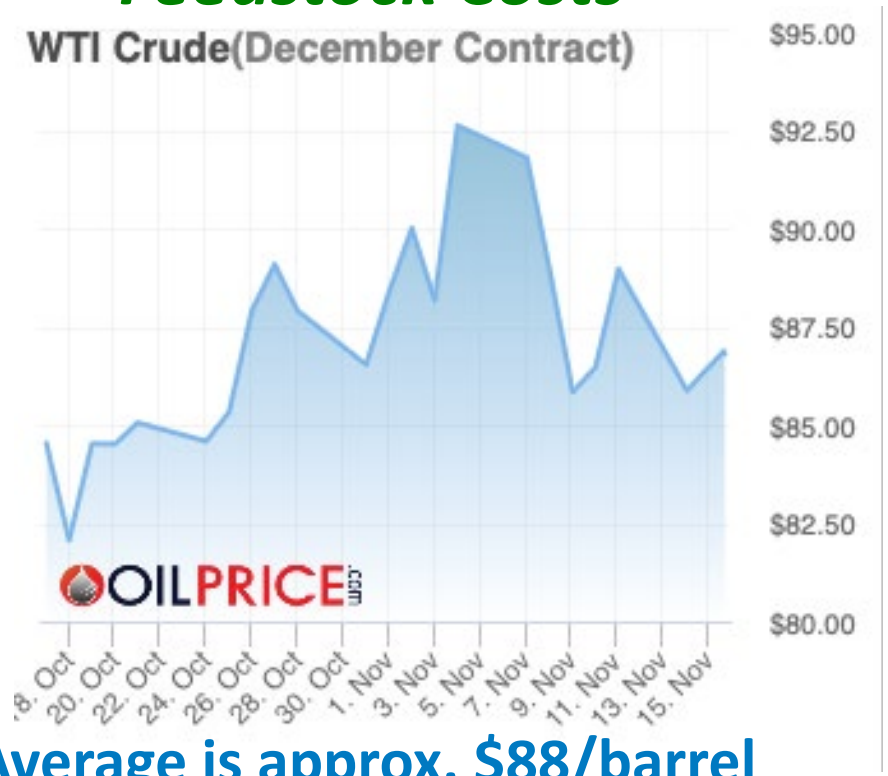
Photo courtesy of istock.com

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***

Why Aren't We Making More Hydrocarbon Biofuels Today?

Feedstock Costs



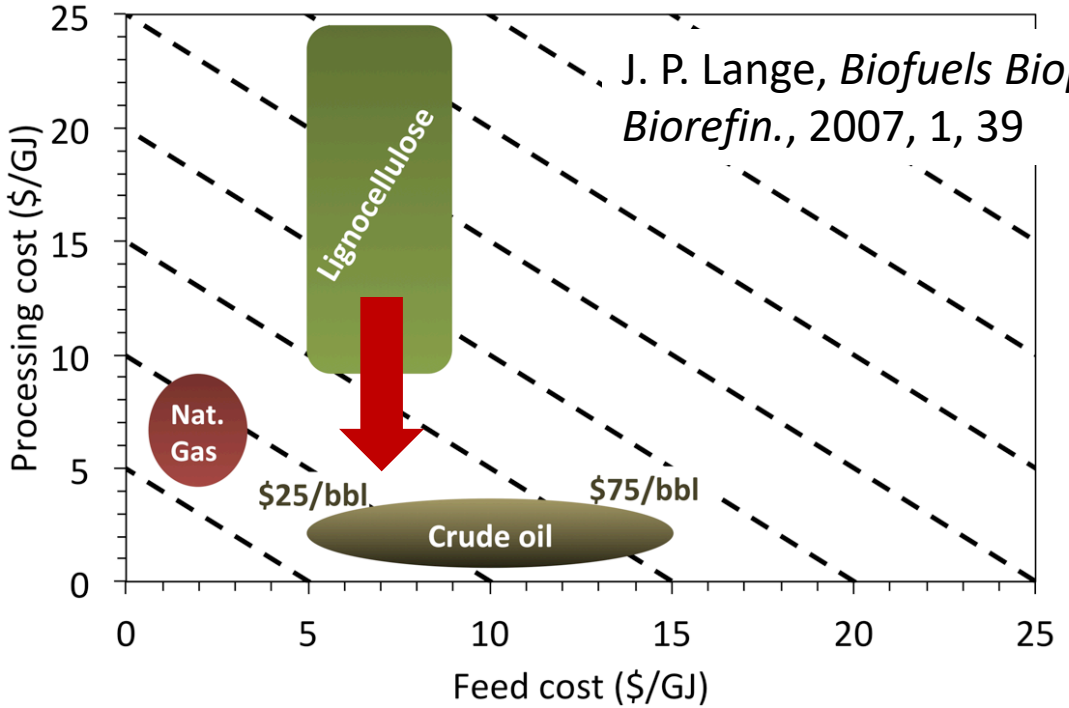
-Average is approx. $88/barrel gives $2.09/gal

Biomass feedstock is $60-100/dry ton

-Assume 50 gal/ton (often 60+ gal/ton)

-Comparable at $1.20-2.00/gal

Processing Costs



-Petroleum refining costs $0.50-0.90/gal gasoline

-Biomass refining costs > $2/gal gasoline

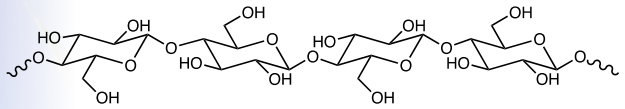
-Realistic biomass-derived fuels > $3/gal

-Catalyst & process development are needed to reduce costs

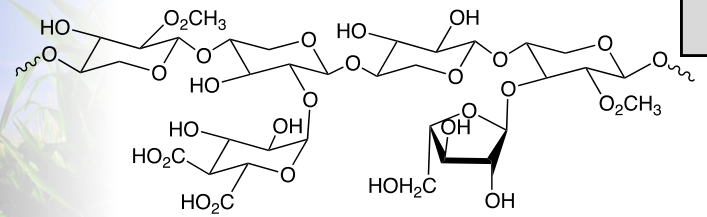
Biomass Grand Challenge: Complex Functionality

Biomass - $CH_{1.4}O_{0.6}$

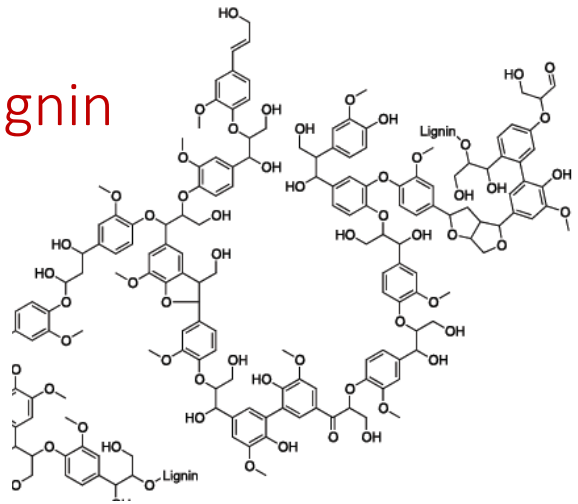
Cellulose



Hemicellulose



Lignin

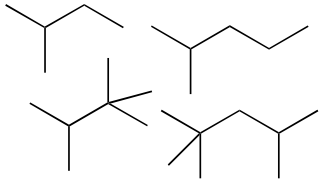


Biochemical and Thermochemical Pathways

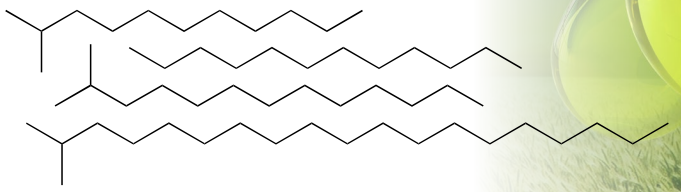
Intermediates
-high yield
-balanced stability and reactivity

Fuels - C_nH_{2n+2}

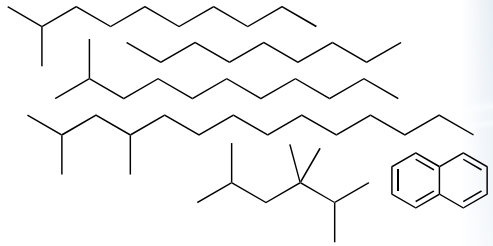
Gasoline

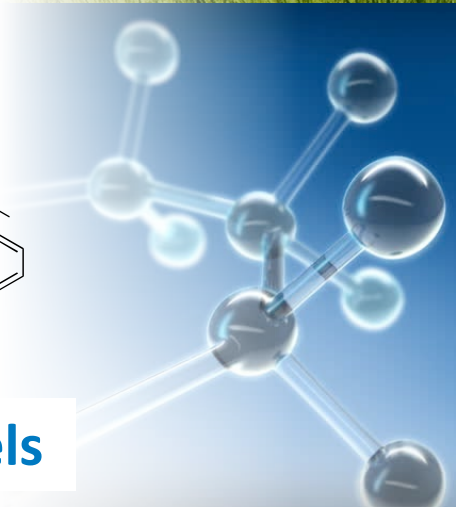


Diesel



Jet Fuel





Multi-functional catalysts are required to convert biomass into fuels

An R&D Consortium Approach to Enable the Bioeconomy

ChemCatBio

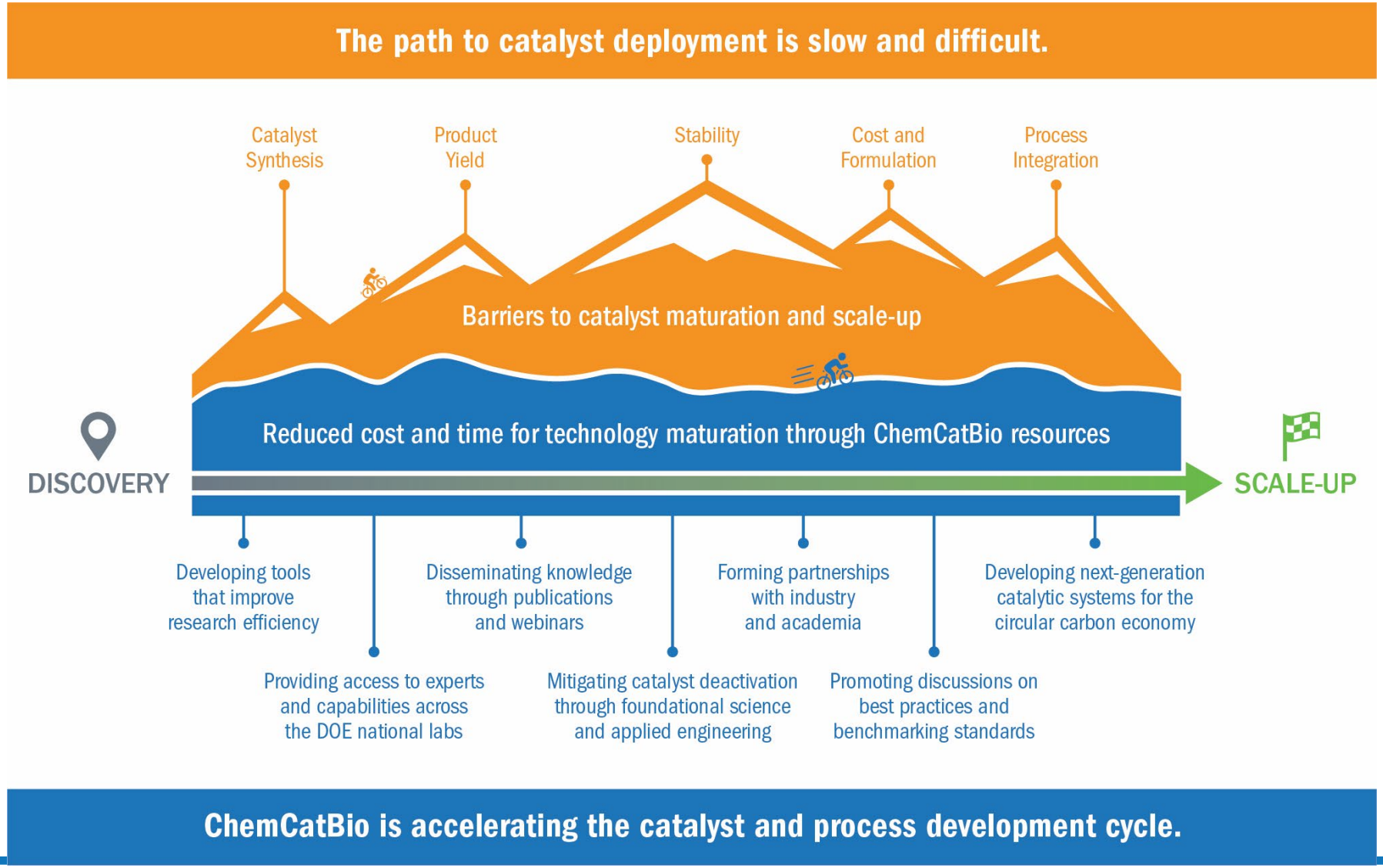
Pursuing the rapid decarbonization of our economy

Accelerating the catalyst and process development cycle for bioenergy applications

chemcatbio.org

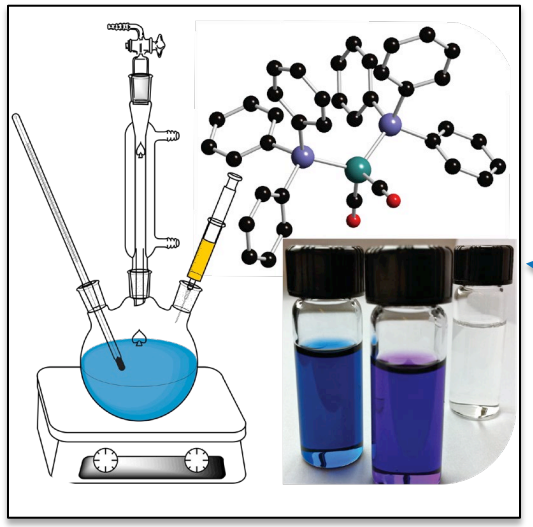
Accelerating Discovery and Development

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

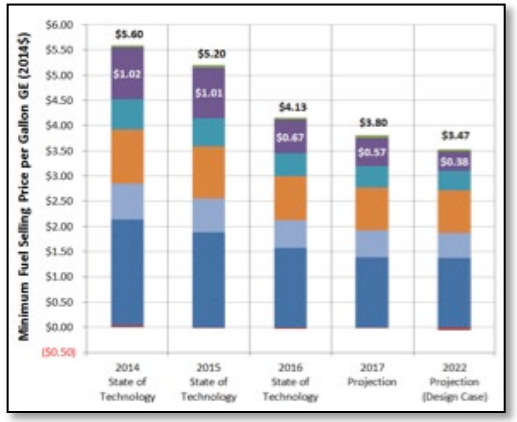


Dual Cycle for Catalyst & Process R&D

Synthesis & Characterization



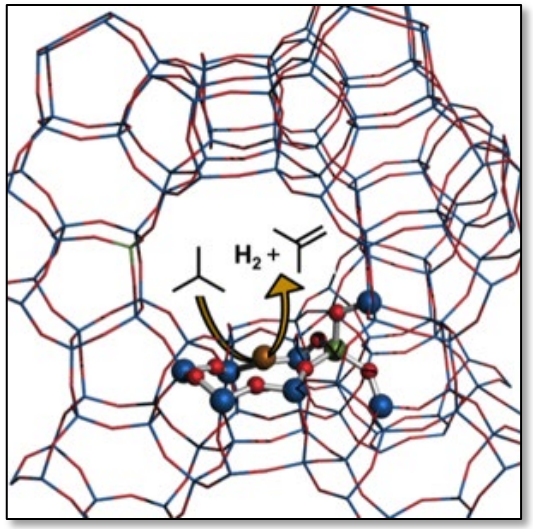
Techno-Economic Analysis (TEA)



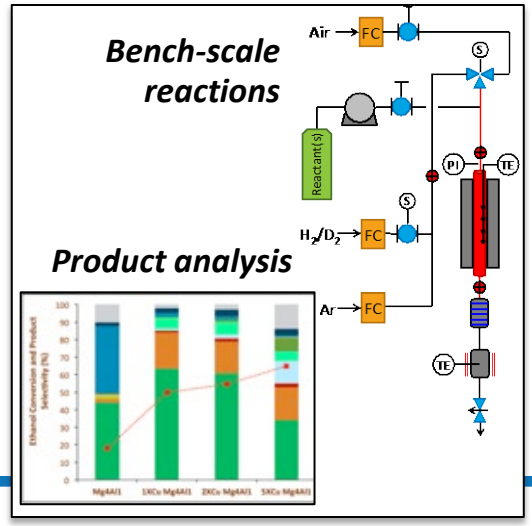
Foundational Catalysis Science

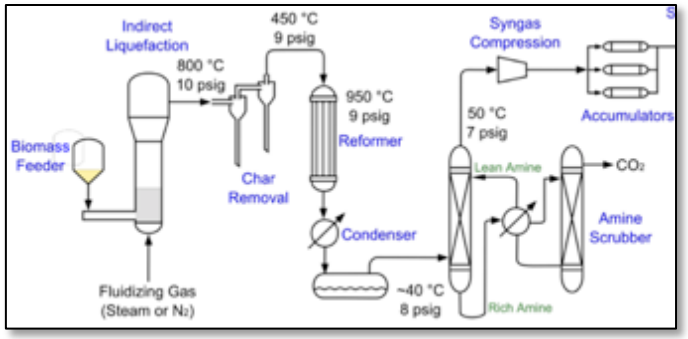
Applied Engineering

Computation



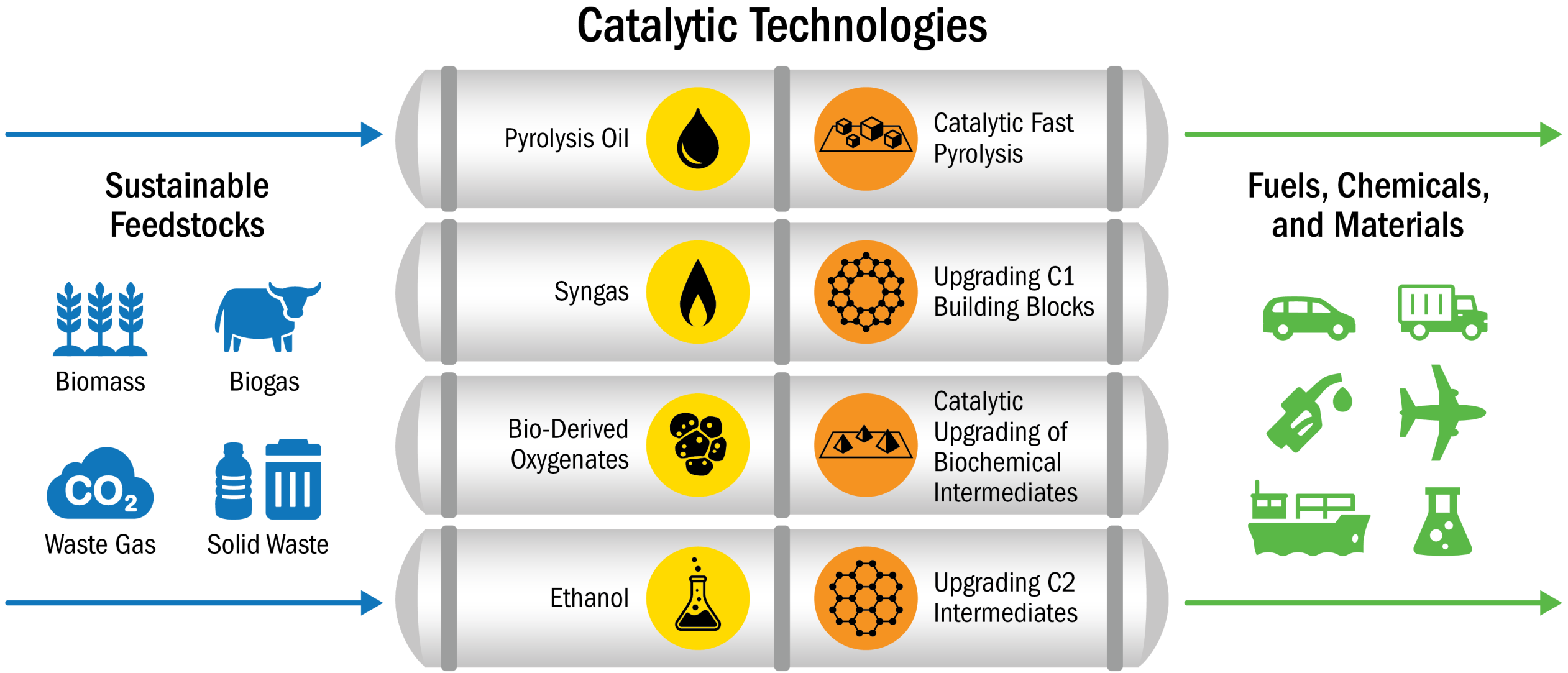
Catalyst Testing





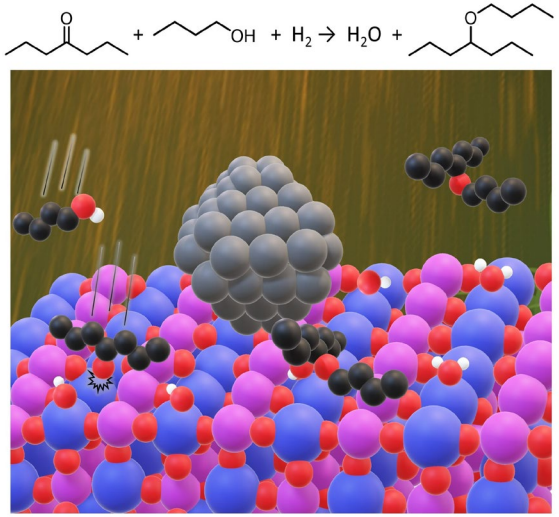
Catalyst Scaling & Process Models

Pathways Under Development in ChemCatBio



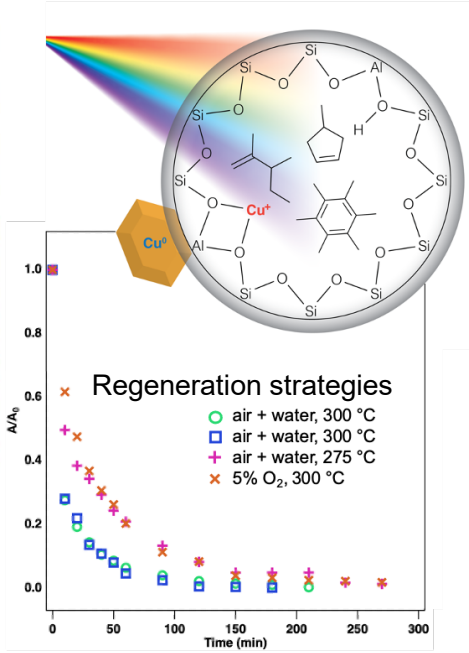
Exploring conversion of multiple feedstocks through multiple processes, targeting SAF as the primary product

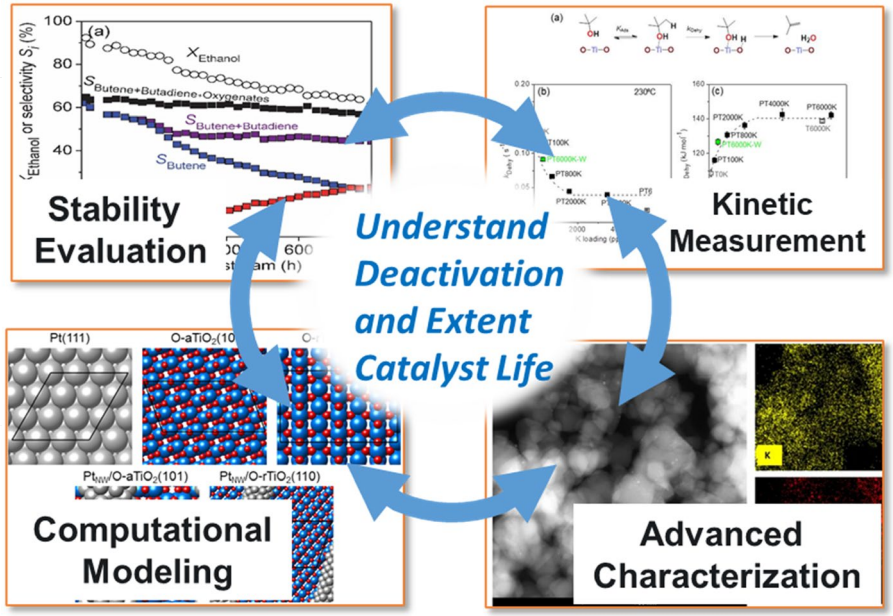
Enabling Capabilities in the Consortium



Computation

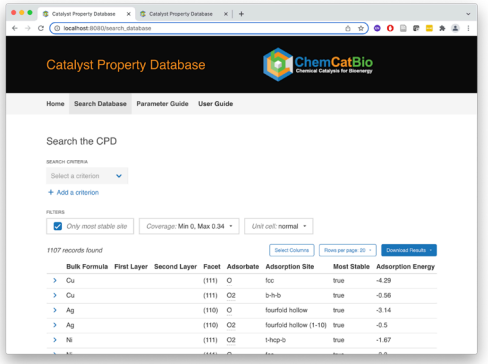
Synthesis & Characterization





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 3 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

For more information, visit chemcatbio.org

WHO WE ARE

>130 researchers

8 DOE National Labs

BETO -sponsored

14 Industry Advisory Board Members

OUR IMPACT

SCIENTIFIC CONTRIBUTIONS

>149 publications

41 h-index since 2016

>4,400 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

9 webinars

Directed Funding Opportunities for industry

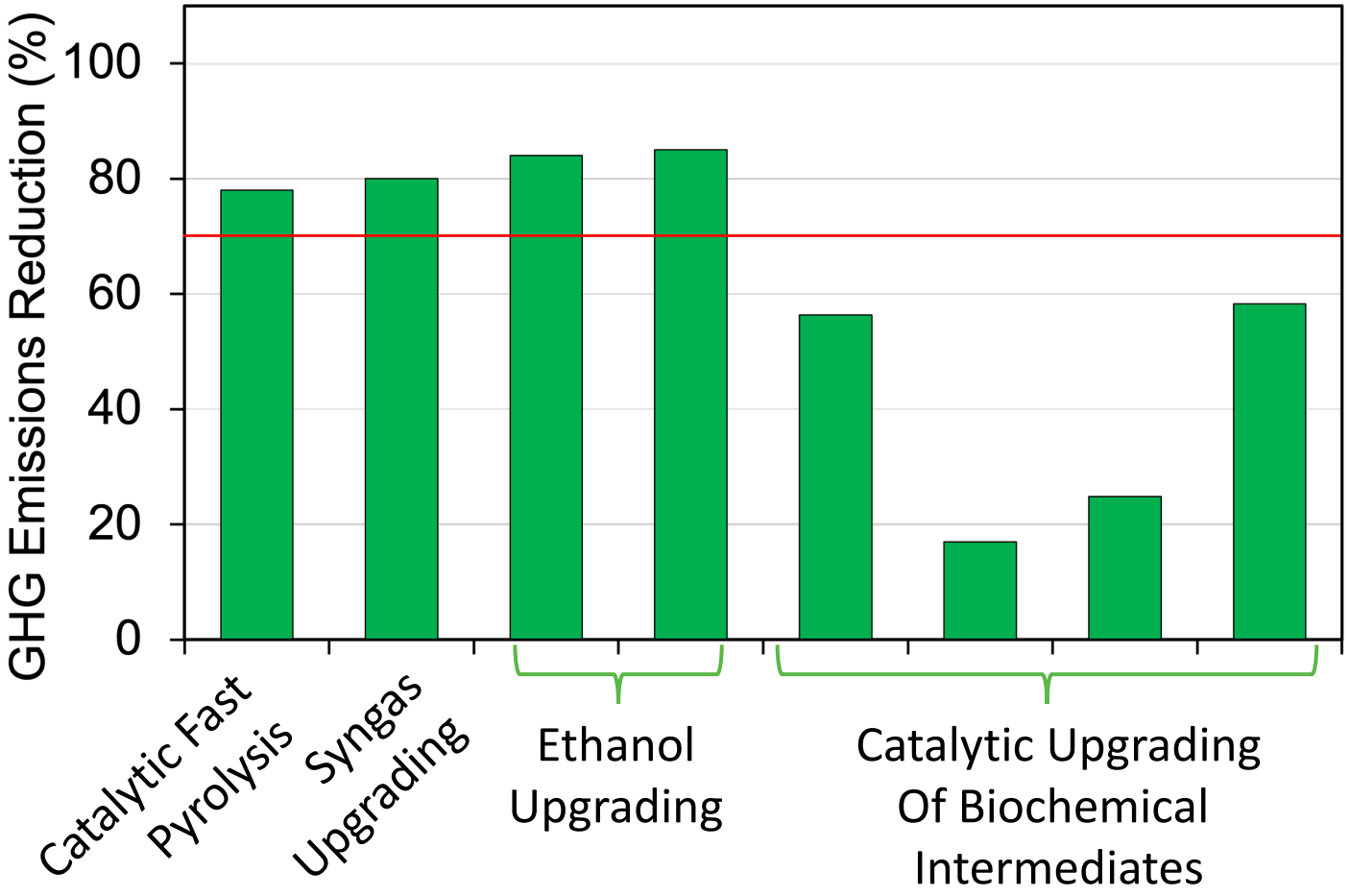
Streamlined access to unique national lab capabilities

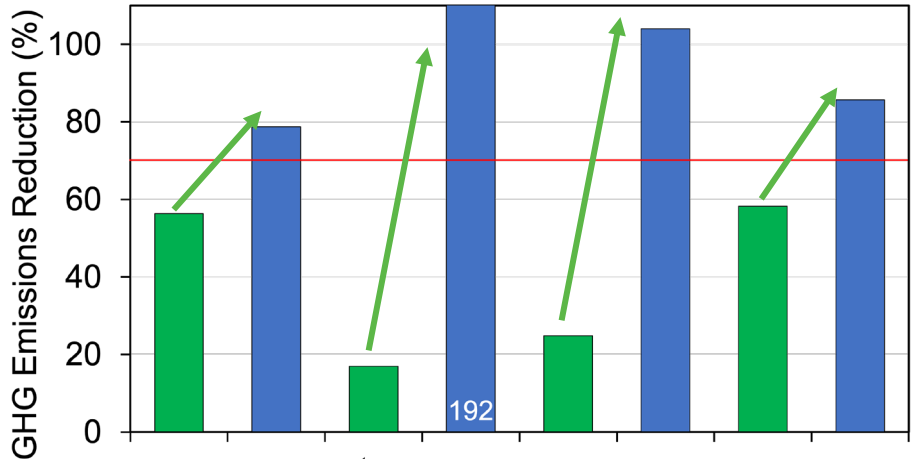
Community Engagement

- 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**

Pathway GHG Emissions Reduction

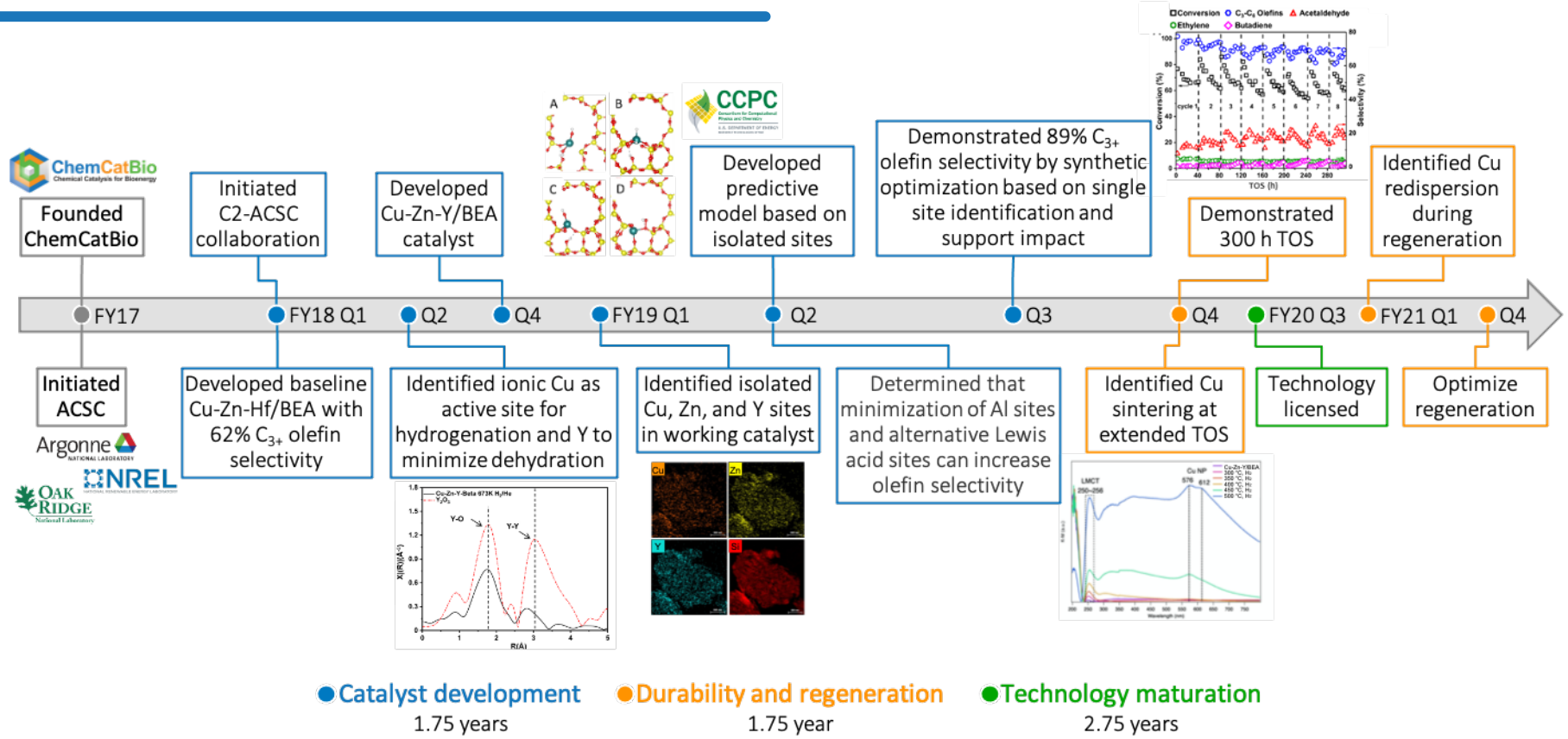
- Multiple pathways exhibit modeled > 70% GHG emissions reduction vs petroleum baseline
- CUBI projects identified future routes to achieve > 70% (e.g., renewable H_2)





Potential reductions from pathways in Catalytic Upgrading of Biochemical Intermediates project

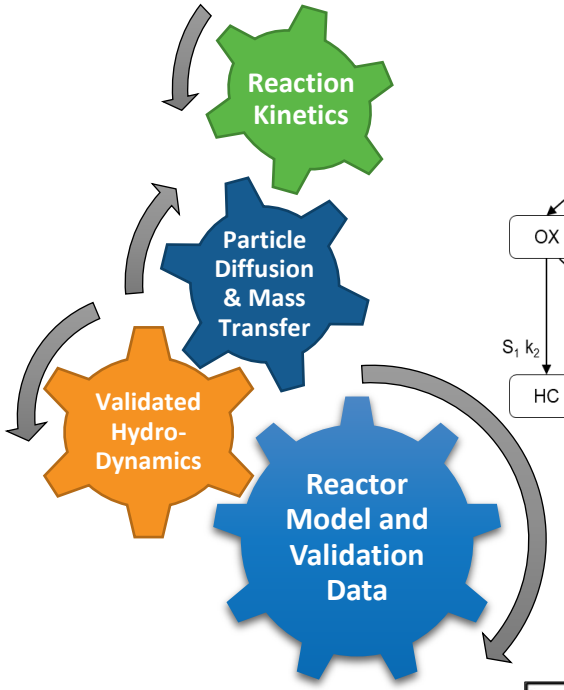
Acceleration of Catalyst and Process Development Cycle

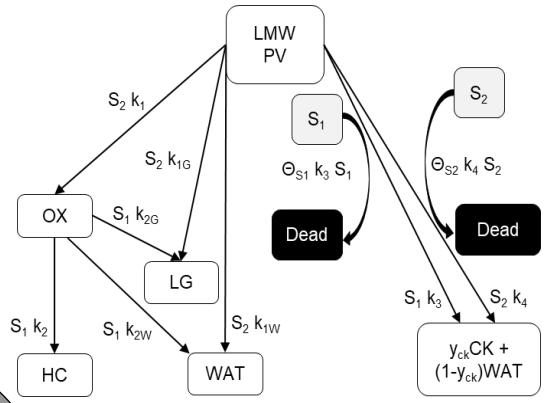


- **Demonstrated a 4x reduction in time** for the **development of a next-gen catalyst** with substantial increase in performance
- In this example, improved C_{3+} olefin selectivity from ethanol was achieved through targeted catalyst design leveraging the **collaborative resources of ChemCatBio**

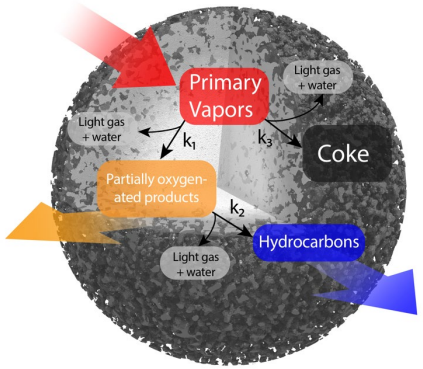
Bioenergy Catalysis Kinetics and Application for Scaleup

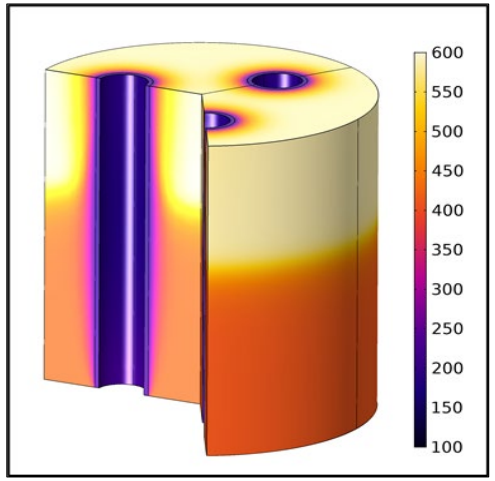
- **Developed a methodology for accurate determination of bioenergy-specific kinetics** and applied kinetics in multiple reactor scale-up models
- Key outcomes:
  - Multicomponent Effectiveness Vector – a new mathematical tool for **analyzing diffusion limitations for cascade reaction mechanisms** in 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

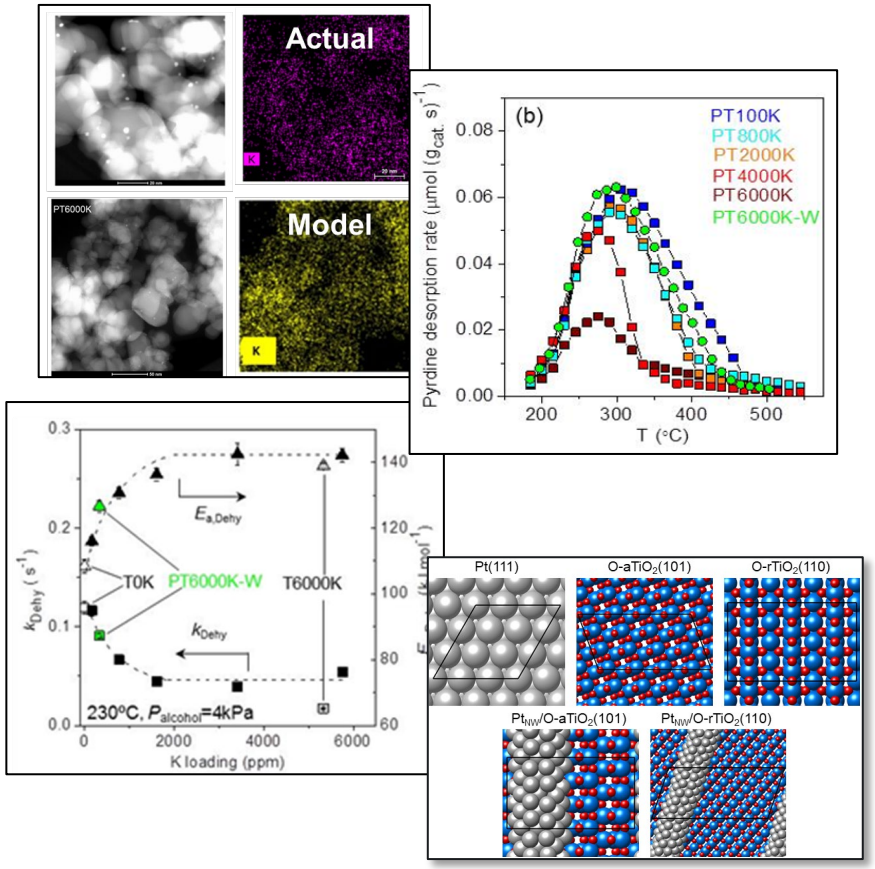
https://www.energy.gov/eere/bioenergy/beto-webinars

Addressing Overarching Catalyst Deactivation Challenges

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

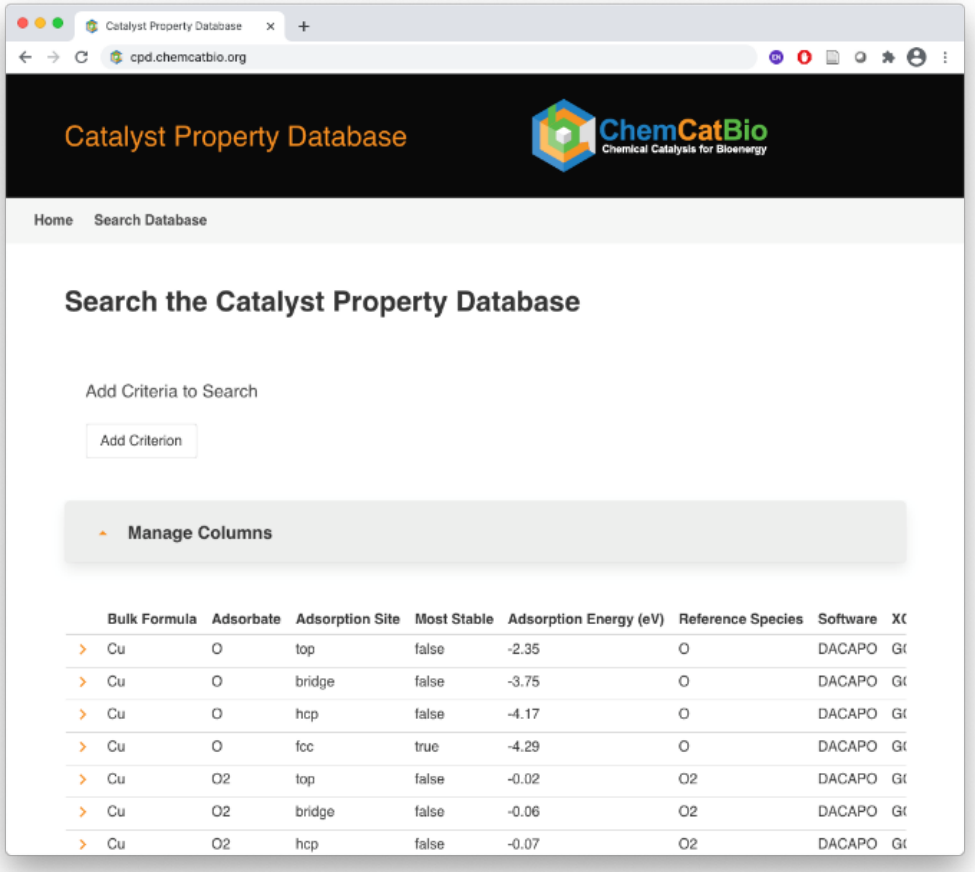
- Developed a comprehensive understanding of the impact of inorganics (K) on different types of active sites on typical multifunction catalysts
  - *ACS Catalysis* **2022**, *12*, 465-480
  - *ACS Catalysis* **2022**, *12*, 13555-13599

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



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

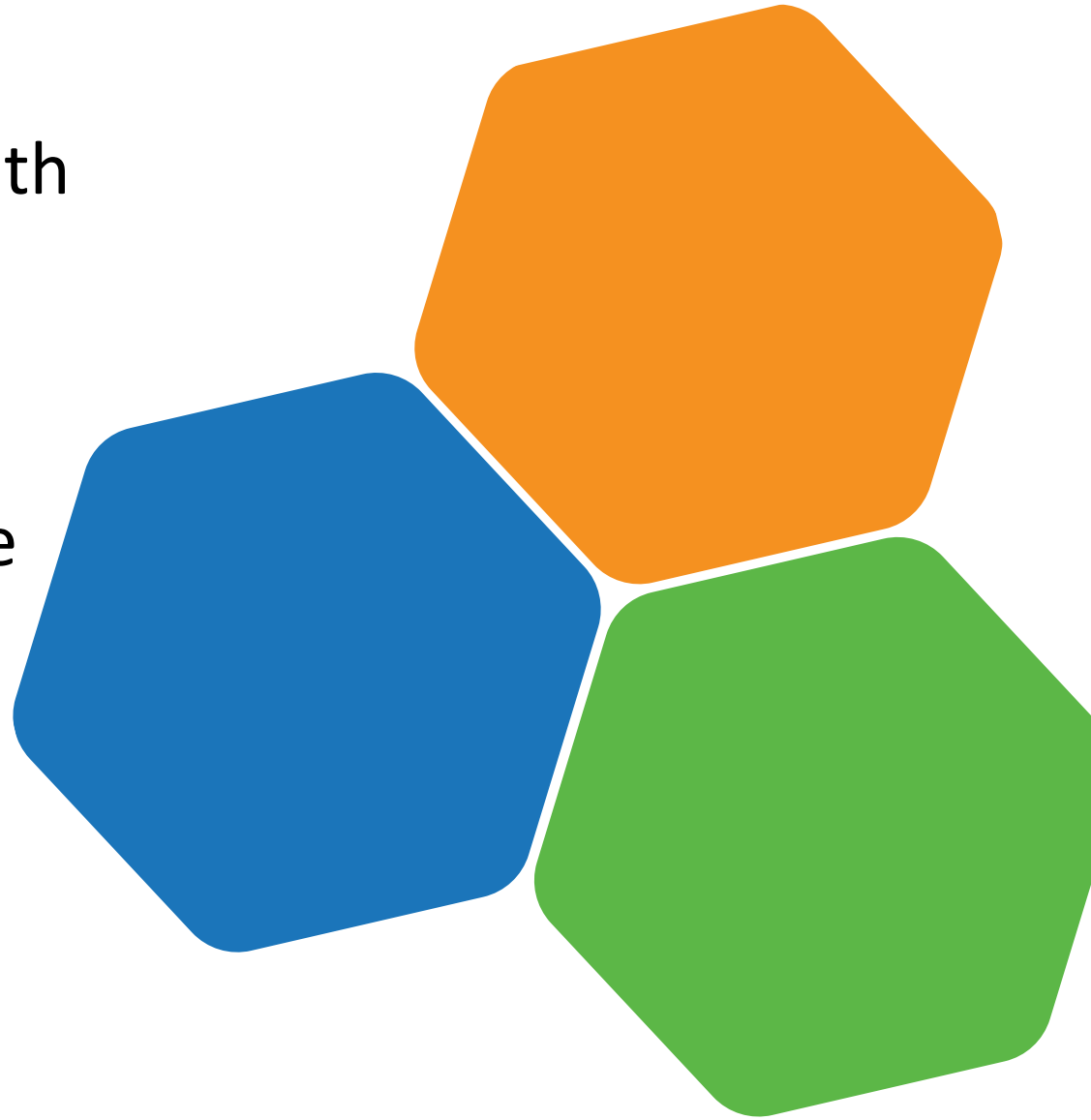
Free and public R&D resource

Consortium Goals for 2023-25

2023-25 Focus Areas

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

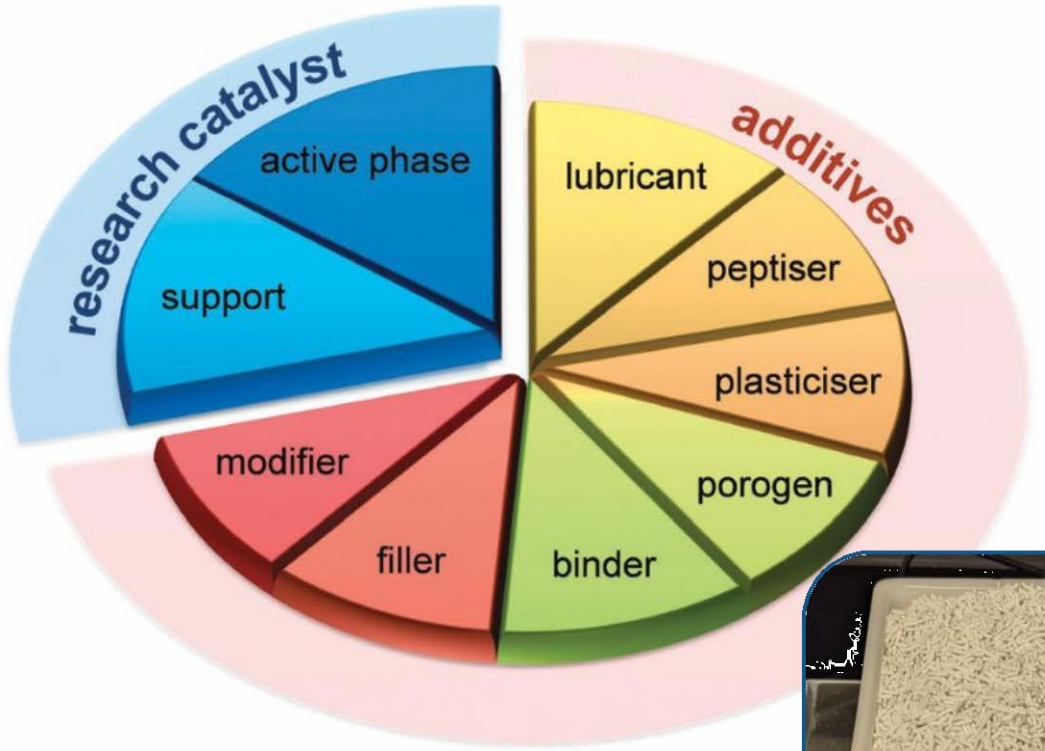
ChemCatBio as a central hub of knowledge for the bioenergy community.



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

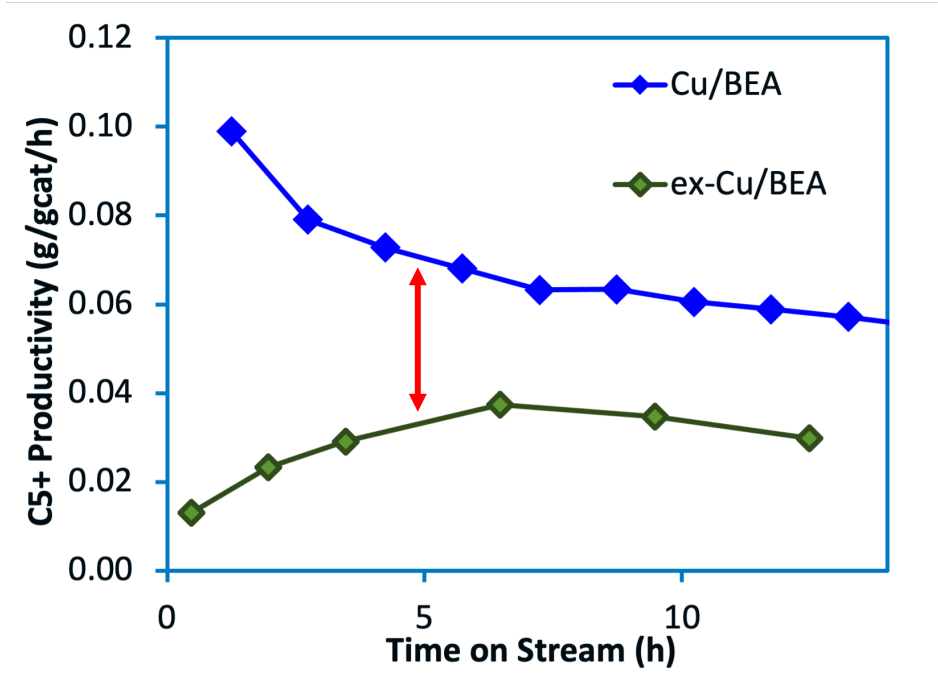
- **Option 2**

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

- **Option 3**

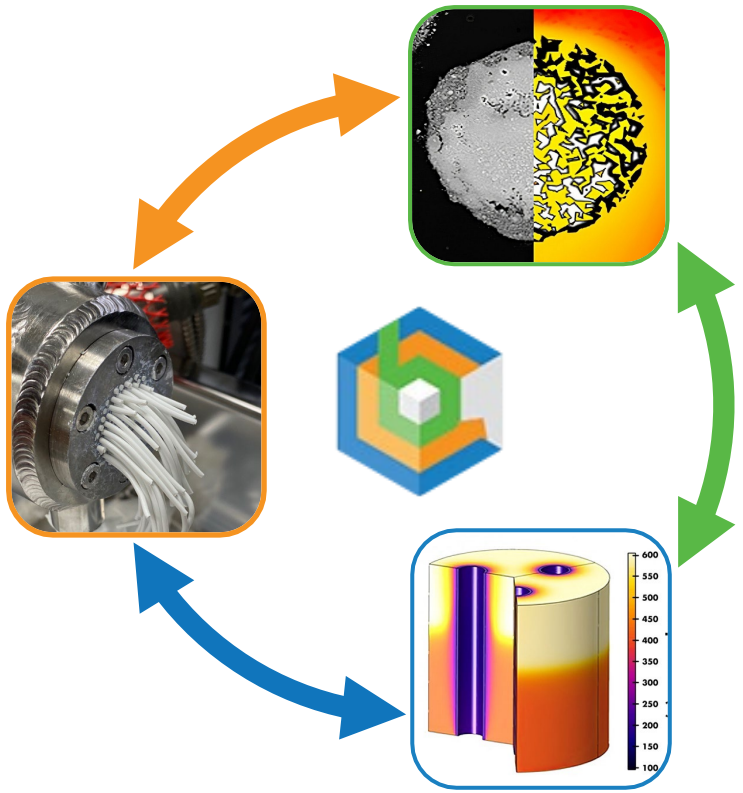
For **pre-commercial catalysts**, develop the **in-house capability** to determine the **structure-property-performance relationships** that inform the transition to engineered forms

- *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 TRL 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

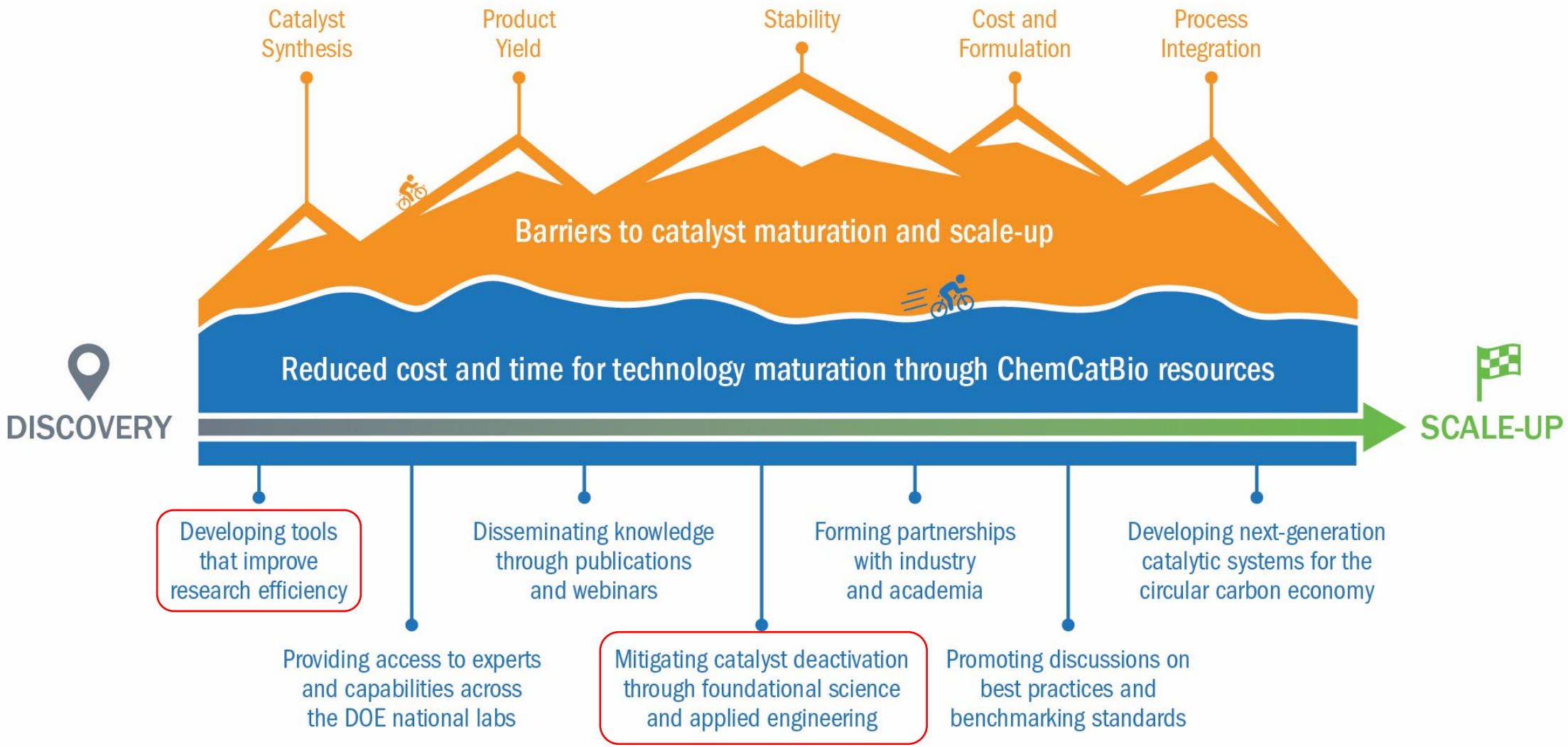


- Addresses the **non-trivial transition** from research to engineered catalysts forms
  - Challenge in maintaining highly-tailored catalyst functionalities
- **Reduces the risk of commercialization** by reducing uncertainty in engineered catalyst operability
  - Loss of activity/selectivity/lifetime 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.

Accelerating Catalyst Design

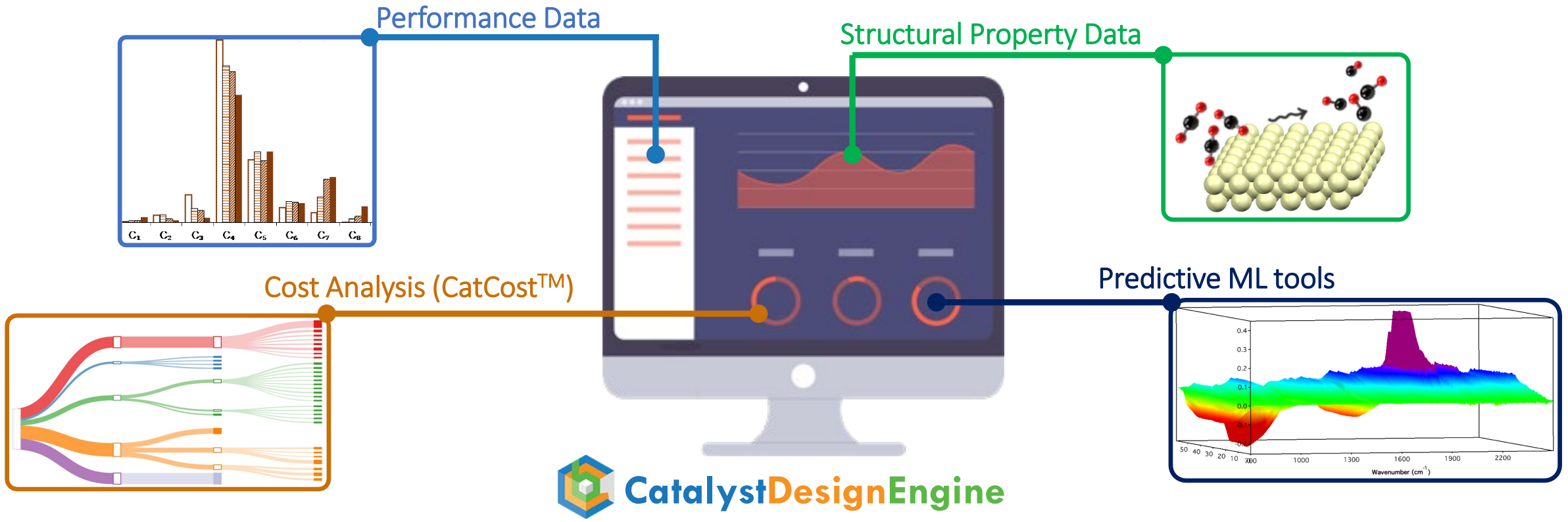
The path to catalyst deployment is slow and difficult.



ChemCatBio is accelerating the catalyst and process development cycle.

Catalyst Design Engine: Vision

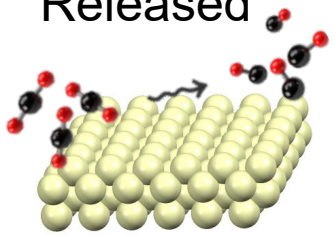
To support and accelerate catalysis RD&D by addressing barriers with a suite of predictive analytical tools



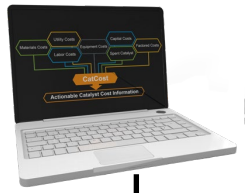
Integrating database technology from **Datahub** with cost estimation from **CatCost** at the **frontier of machine learning** to transform catalyst design and deployment

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

Mitigating the Risk of Deactivation

A Critical Knowledge Gap: Catalyst Stability

Problem

Among the three “virtues” of catalyst performance (activity, selectivity, and stability), **stability is the least explored**

➡ Biomass-derived feedstocks bring unique and challenging catalyst deactivation issues

Proposed Solution

Create a catalyst deactivation mitigation resource with targeted insights, techniques, and tools

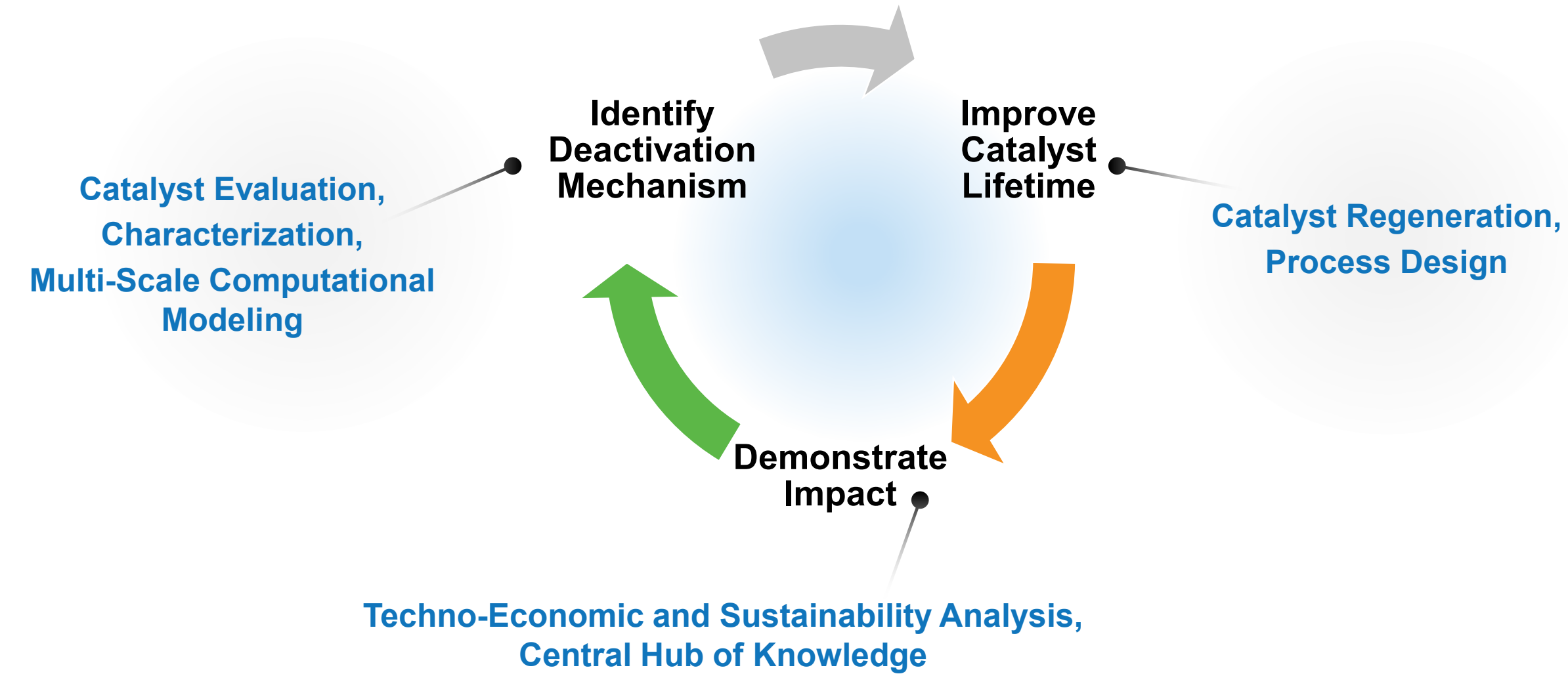
Overarching Catalyst Deactivation Challenges

Interwoven challenges affect catalyst durability in many biomass conversion pathways

How can CCB address these overarching challenges?

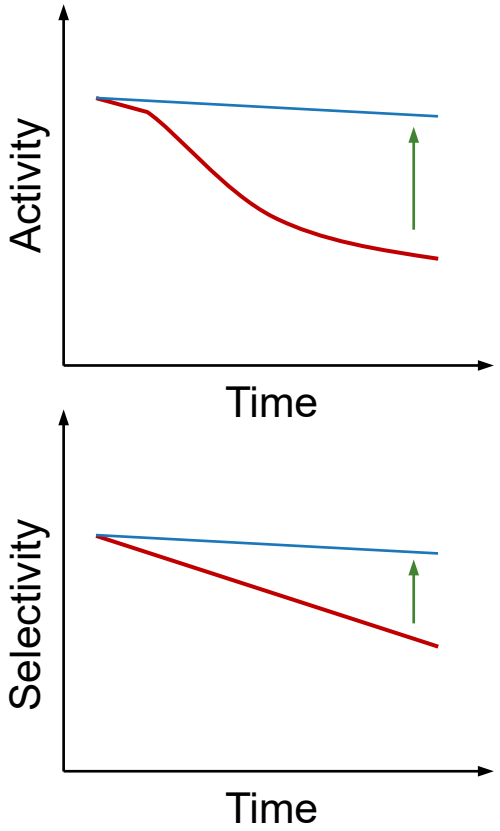
- ***Coke***: determine properties, distribution, removal (combustion kinetics)
- ***Contaminants***: determine distribution, interaction with active sites
  - Provide database on catalyst properties and interaction with contaminants
- ***Water***: build upon existing literature, but with specificity to biomass feedstocks and conversion processes

ChemCatBio Approach Leverages our Unique Capabilities



Our Goals for Deactivation R&D

- Advance our technologies **towards commercialization** and **generate knowledge that can translate** to industry
- Identify the overarching catalyst deactivation issues associated with **specific biomass feeds**
- **Establish a set of laboratory-accessible tools/techniques** to evaluate stability and make improvements.
- **Avoid pitfalls during technology maturation** by increasing awareness about deactivation challenges in early-stage research



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)

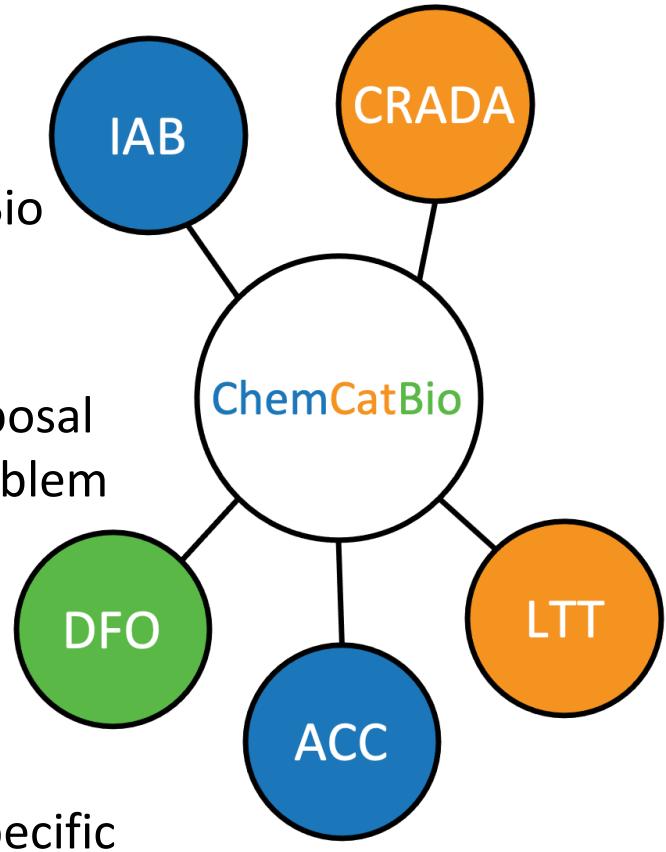
- Funds from BETO to generate a new ChemCatBio project based on a joint proposal between industry and ChemCatBio researchers to solve a specific industry problem

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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Technology Briefs and Newsletter

- **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/technology-briefs.html

- **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/news-archive.html

Summary

- Catalysis will play an enabling role in decarbonizing the fuel and chemical sectors
- Biomass as a feedstock introduces unique challenges for catalytic technologies
- ChemCatBio seeks to accelerate the catalyst and process development cycle to help shorten the time to market for renewable technologies

Learn more and subscribe to our newsletter (The Accelerator) at chemcatbio.org

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ChemCatBio
Chemical Catalysis for Bioenergy

Energy Materials Network
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Thank you. Let's Discuss.

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Access the CPD: https://cpd.chemcatbio.org/

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