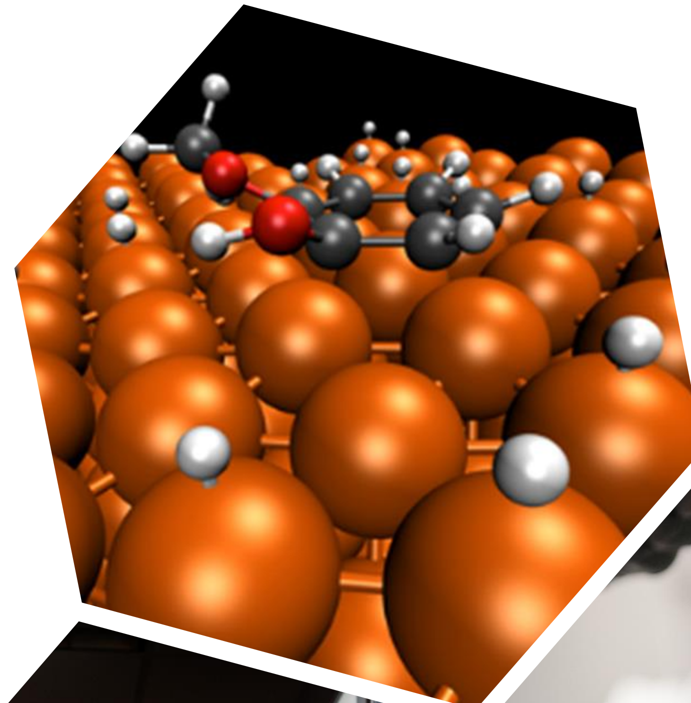
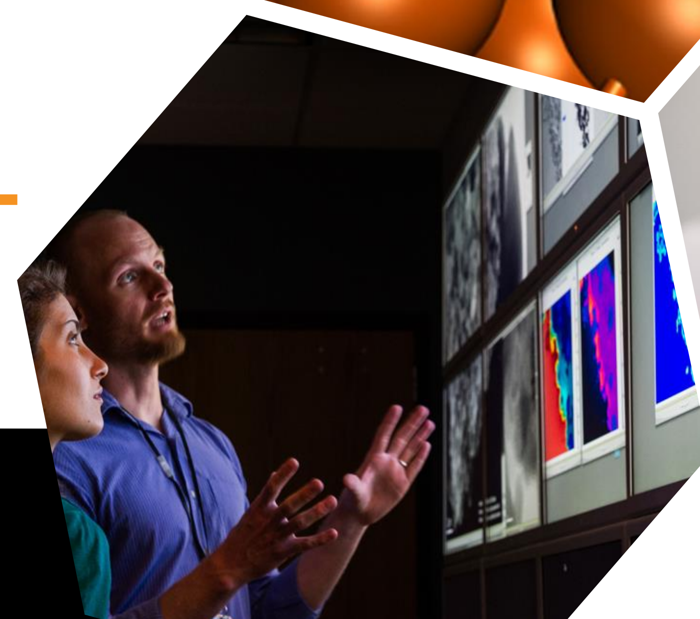
ChemCatBio
Chemical Catalysis for Bioenergy

DOE Bioenergy Technologies Office (BETO) 2019 Project Peer Review

Overview of the Chemical Catalysis for Bioenergy Consortium

Josh Schaidle





Catalytic Upgrading

March 2019

Goal Statement

Goal: ***Overcome catalysis challenges*** for the conversion of biomass and waste resources into fuels, chemicals, and materials by leveraging unique U.S. DOE national lab capabilities

Outcome: ***Accelerate the catalyst and process development cycle for bioenergy technologies***, leading to enhanced energy security and national leadership in the global bioeconomy

- Collaborative, multi-national lab approach targeting both pathway-specific and overarching catalysis challenges
- Engagement with industry to identify knowledge gaps and tackle critical industry-relevant challenges that can be addressed through early-stage R&D
- Leverage world-class capabilities in modeling, synthesis, characterization, integrated catalyst/process evaluation, and economic analysis

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

Overview: Historical Motivation

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

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*

Energy Materials Network
U.S. Department of Energy

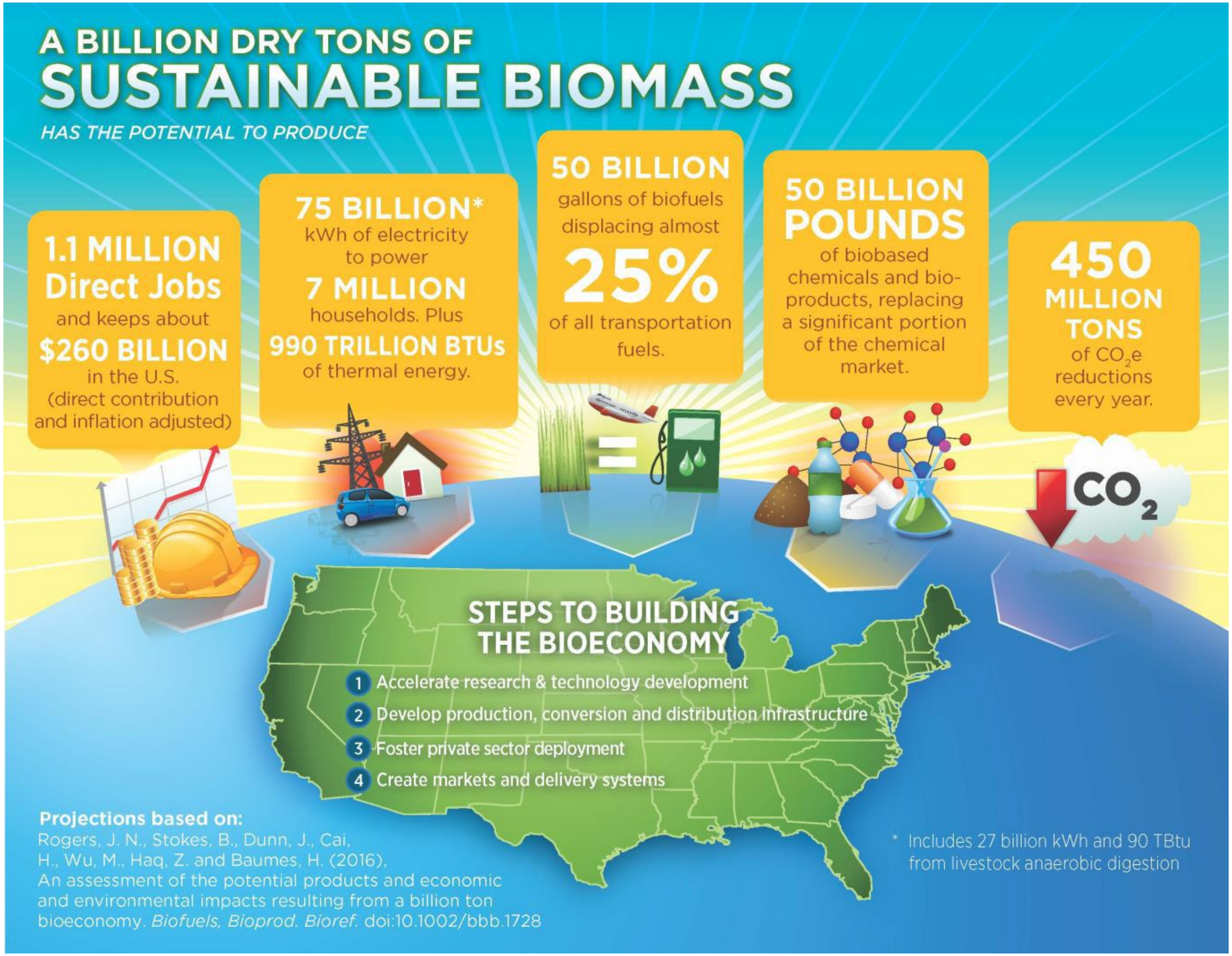
Goal: *Accelerate the development of advanced materials for clean energy applications*

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

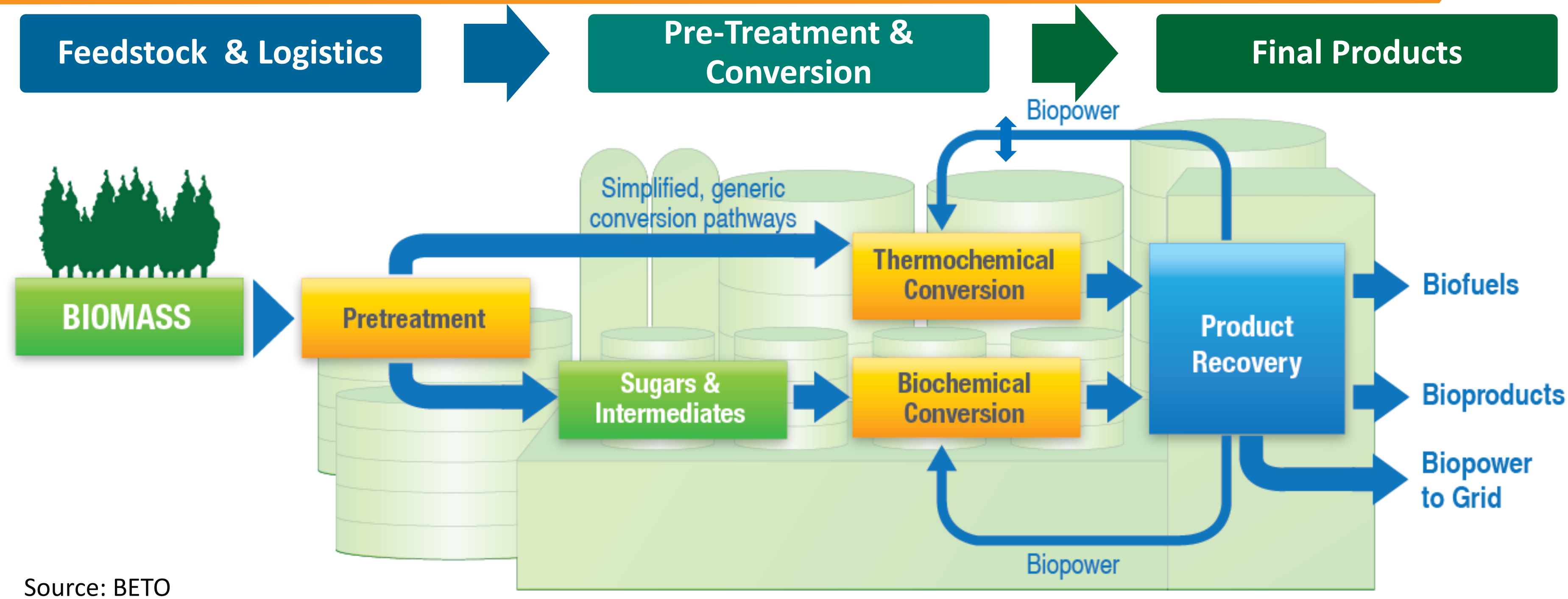
ChemCatBio
Chemical Catalysis for Bioenergy

[Launched at start of FY17]

Overview:
Potential Impact of a Billion-Ton Bioeconomy



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



Source: BETO

Key Catalytic Bioenergy Processes	Challenges due to Biomass Composition
• Catalytic Upgrading of Biological Intermediates • Synthesis Gas Upgrading • Catalytic Fast Pyrolysis • Catalytic Upgrading of Aqueous/Gaseous Waste Streams • Catalytic Hydroprocessing • Lignin Deconstruction and Upgrading	• 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

Catalyst cost can contribute up to 10% of the biofuel production cost

Project Overview: Value Proposition

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

Objectives and *Success Factors*:

- Demonstrate catalytic advancements that result in reduced conversion costs for key BETO pathways (indirect liquefaction, catalytic fast pyrolysis, and biochemical routes), targeting $3/GGE MFSP by 2022
- Provide early-stage R&D to enable BETO 2022 engineering-scale verification
- Demonstrate accelerated catalyst-process development cycle
- Enable accelerated market adoption by facilitating industry/stakeholder access to our capabilities, establishing industry partnerships and advisory board, and developing tools to improve research efficiency

Differentiators:

- Working with realistic process streams (woody biomass, fermentation broth)
- Targeting both pathway-specific and overarching catalysis challenges
- Leveraging world-class national lab capabilities and expertise
- Guiding R&D with TEA and input from industry advisory board

Management Approach: Consortium Structure

BETO
Nichole Fitzgerald

Industry and Academic Partners

Director
Josh Schaidle

- Single point of contact
- Portfolio management
- Strategic initiatives

Key Interactions

- Biannual face-to-face meetings
- Biweekly teleconferences
- Quarterly teleconferences with IAB

Steering Committee
28 PI's and Co-PI's

- Coordinate and lead R&D
- Provide technical guidance
- Identify unique lab capabilities
- Serve in specific roles

Industry Advisory Board
8 members

- Guide the consortium toward industry-relevant R&D
- Provide a business perspective
- Identify knowledge gaps

Team
100+ contributors

Technical Capabilities Experts | *Technology Transfer Experts* | *Data Experts*

Management Approach: ChemCatBio Foundation

Integrated and collaborative portfolio of catalytic technologies and enabling capabilities

Catalytic Technologies

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

*FY19 Seed Project

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)

Technical Approach:
Foundational Catalyst-Process Development

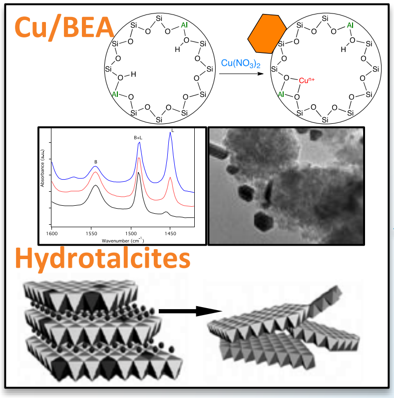
Foundational Science

Enables hypothesis-driven catalyst design

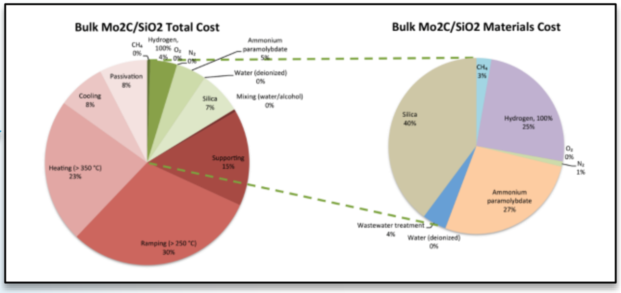
Applied Engineering

Enables evaluation of key process metrics and deactivation

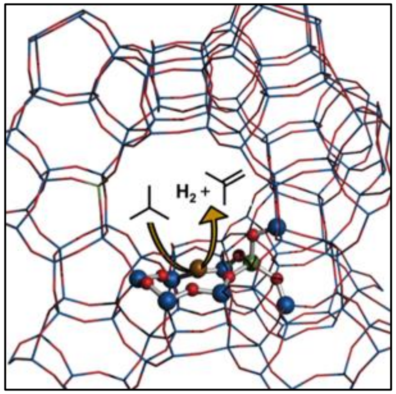
Advanced Synthesis and Characterization



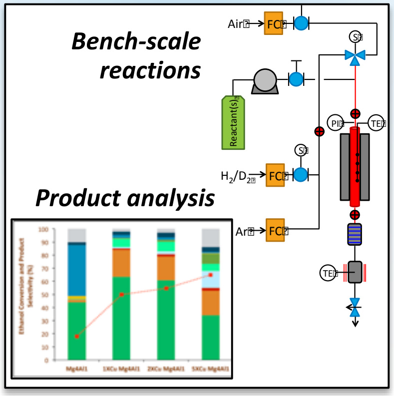
Catalyst Cost Estimation

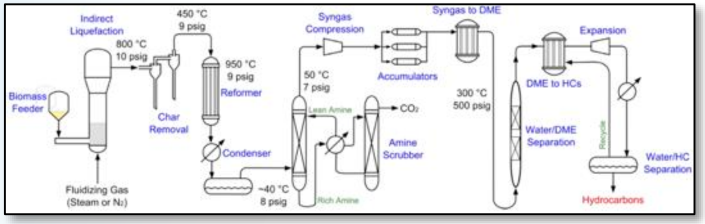


Theory



Performance Evaluation





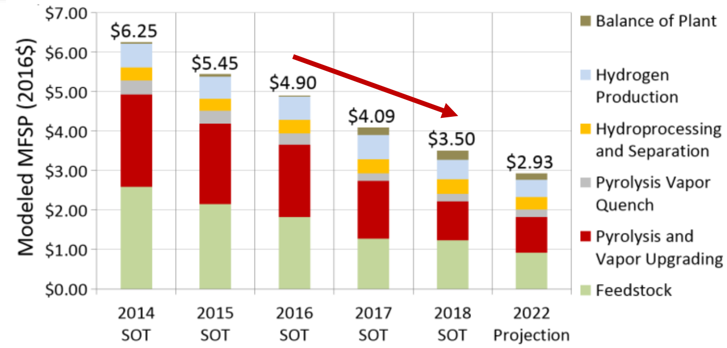
Catalyst Scaling and Integrated Testing

Progress: Technical Accomplishments
Addressing pathway and overarching challenges

Catalytic Fast Pyrolysis (CFP)

***Challenge**:* Low carbon efficiency for CFP

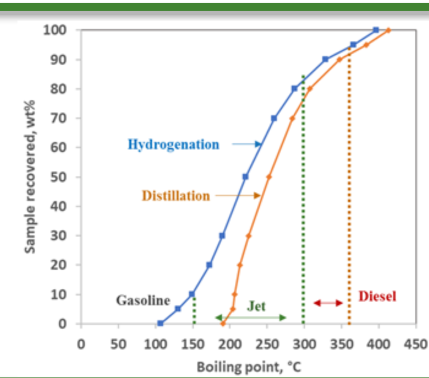
***Accomplishment**:* Improved CFP C efficiency from 33% (2016) to 45% (2018) through catalyst and process development, resulting in $1.4/GGE reduction in MFSP



Catalytic Upgrading of Biochemical Intermediates

***Challenge**:* Generating high-quality distillate fuels

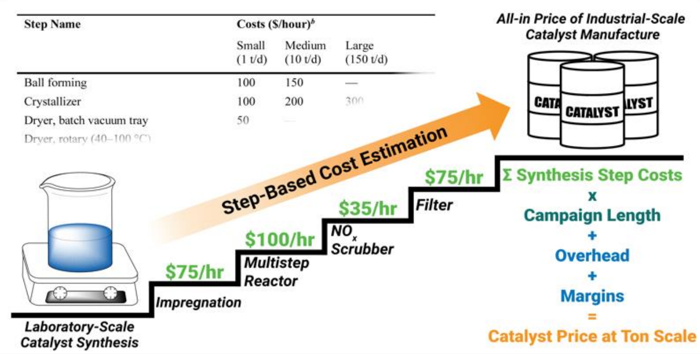
***Accomplishment**:* Demonstrated distillate fuel production starting from three different intermediates (butyric acid, 2,3-butanediol, and furfurals), with specific products having high cetane numbers (e.g., 49)



Catalyst Cost Model Development

***Challenge**:* Linking catalyst cost and performance

***Accomplishment**:* Developed and released a first-of-its-kind, industrially-vetted, publicly-available tool for estimating the cost of pre-commercial catalysts *(CatCost)*

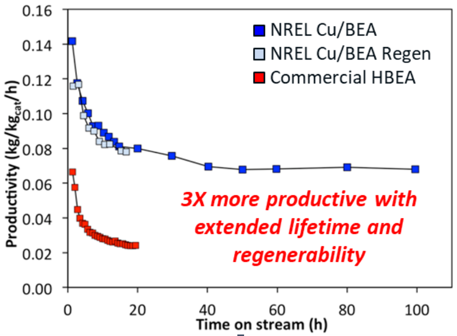


Progress: Cross-Consortium Collaboration Develops Next-Generation Catalysts with Improved Selectivity

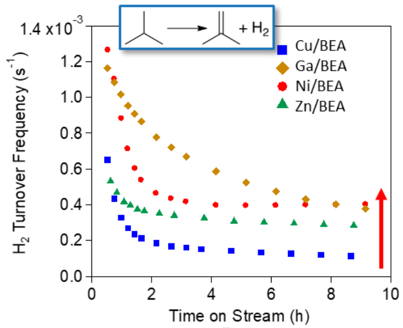
Demonstrated Full Catalyst-Process Development Cycle

Core Catalytic Technology (IDL-NREL)

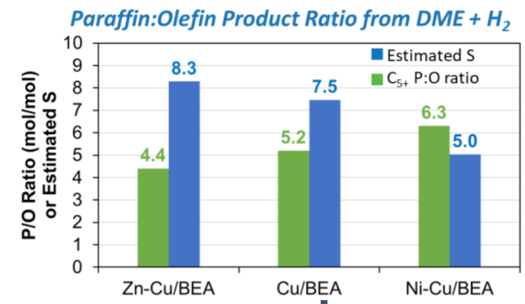
Developed catalyst that outperformed commercial HBEA for high-octane gasoline production



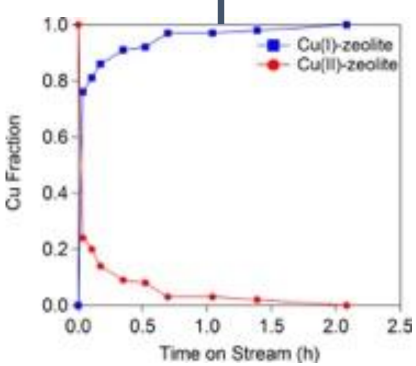
Evaluated computationally-predicted materials



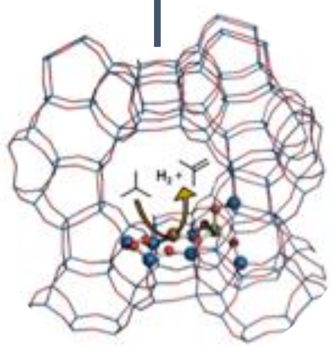
Verified improved selectivity control with bimetallic formulations



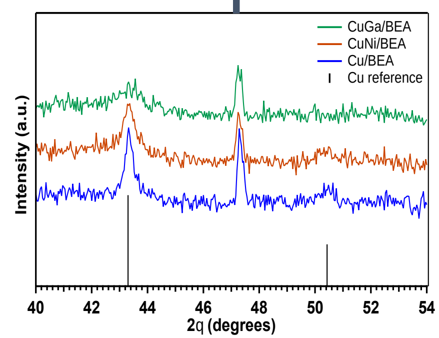
Controlling Paraffin:Olefin Ratio for DME Homologation Enables Control of Fuel Properties



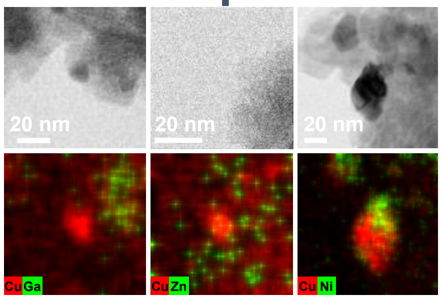
Identified Cu(I) as active site for dehydrogenation (ACSC-ANL)



Predictive model for dehydrogenation (CCPC-NREL)



Synthetic control of speciation in bimetallic catalysts (ACSC-NREL)



Determined speciation in working catalysts (ACSC-ORNL)

Enabling Capabilities

Progress: Industry and Stakeholder Engagement

Held Stakeholder Listening Day in June 2017 in conjunction with North American Catalysis Society Meeting

- Attended by 25 experts across catalysis and bioenergy eco-system
- Focused on shaping ChemCatBio value proposition and developing ways to engage with industry and academia
- Compiled a report with key feedback and action items

Specific Feedback: Need to build awareness of ChemCatBio

Outcome:

- Initiated a public webinar series (presentations posted to website)
- Host annual ChemCatBio symposium at ACS National Meeting
- Maintain up-to-date website

Established an industry advisory board with 8 members across the catalysis and bioenergy value chains

- Members currently or formerly at Honeywell UOP, Chevron, Andeavor, Johnson Matthey, Valmet, Dow, Merck, and PTI Global Solutions
- Meet quarterly via teleconference to discuss progress and solicit feedback

Specific Feedback: Critical need to understand deactivation and utilize world-class synthesis/characterization capabilities

Outcome:

- Initiated a new enabling capabilities project in FY19 focused on deactivation
- Incorporated neutron scattering and MOF synthesis into ACSC in FY19

Progress: Industry Partnerships

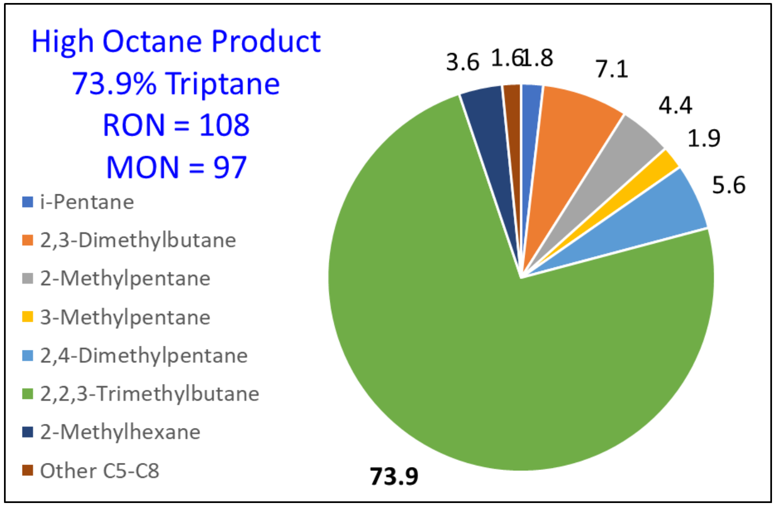
Established 10 new industrial partnerships through competitive projects that leverage ChemCatBio capabilities and expertise to overcome catalysis challenges

- Leveraging ChemCatBio capabilities in synthesis, characterization, evaluation, and modeling
- Diverse slate of feedstocks (biomass and waste streams), conversion approaches, and products

gevo · BIGOX ENERGY · Visolis (Carbon Negative Materials) · Vertimass (Transformative fungible biofuels.) · OPUS 12 · LanzaTech (capturing carbon. fueling growth.) · SIRONIX RENEWABLES · JM Johnson Matthey (Inspiring science, enhancing life) · ALD nanosolutions

Indirect Liquefaction: Partnered with Enerkem through TCF to generate high-octane gasoline at pilot-scale from MSW-derived methanol

- Prepared 20kg batches of proprietary Cu/BEA catalyst developed within ChemCatBio
- Produced 20L of high-octane gasoline
- Achieved 500h TOS



Relevance: Bioenergy Industry

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

- Tackling ***overarching catalysis challenges while working with real process streams*** has the potential to broadly enable the bioenergy industry
  - ChemCatBio R&D guided by TEA and stakeholder/IAB input
  - Examples: Understanding and mitigating deactivation (structure-stability relationships), controlling active phase (metal-support interface, metal-zeolite)
- ChemCatBio and BETO held a ***Directed Funding Opportunity*** in FY17 to enable industry to leverage ChemCatBio capabilities and expertise
  - Industry-led proposals ***requested more than 2x available resources***
  - Example value proposition for industry – ***access to tools and expertise***:

"The collaboration with NREL provides extremely valuable industrial validation to the emerging applications for advanced catalyst thin film coatings. … ***We do not have ready access to such tools and expertise as a company****. … The conversion demonstration and techno-economic modeling generate* ***key de-risking data to show how improved catalyst durability with ALD can impact the bottom line****."*

- Karen Buechler, CTO

ALD nanosolutions

Relevance: Reducing Biofuel Production Costs

Reducing biofuel production costs through advancements in catalysis, resulting in technology pathways that meet or exceed BETO's 2022 MFSP goal of $3/GGE

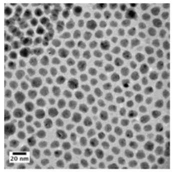
- MYP technical barriers to achieving BETO's goal of $3/GGE by 2022:
  - Improving catalyst lifetime
  - Increasing the yield from catalytic processes
  - Decreasing the time and cost to developing novel industrially relevant catalysts
- ChemCatBio is actively addressing these barriers for three key pathways (indirect liquefaction, catalytic fast pyrolysis, and biochemical routes) by:
  - Developing an integrated and collaborative portfolio of catalytic technologies and enabling capabilities
  - Leveraging world-class, national lab capabilities in modeling, synthesis, characterization, integrated catalyst/process evaluation, and economic analysis
  - Targeting both pathway-specific and overarching catalysis challenges while working with real-world process streams

Future Work: Tool Development and Utilization

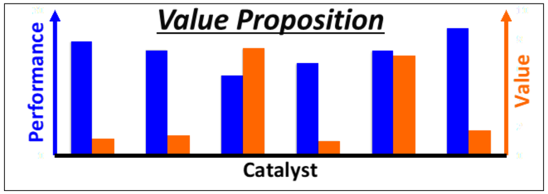
Expand the development and utilization of tools that improve research efficiency and accelerate the catalyst-process development cycle

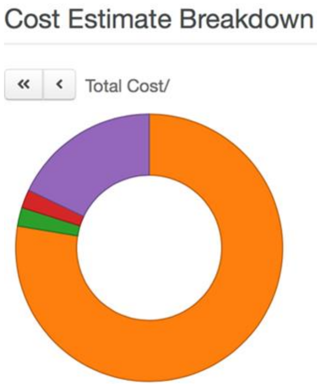
Expand utilization of the CatCost tool and solicit feedback on desirable features and updates

- Work with universities to incorporate *CatCost* into their curriculum for engineering and catalysis courses
- Reach out to users to get targeted feedback for future updates
- Outreach at conferences and seminars



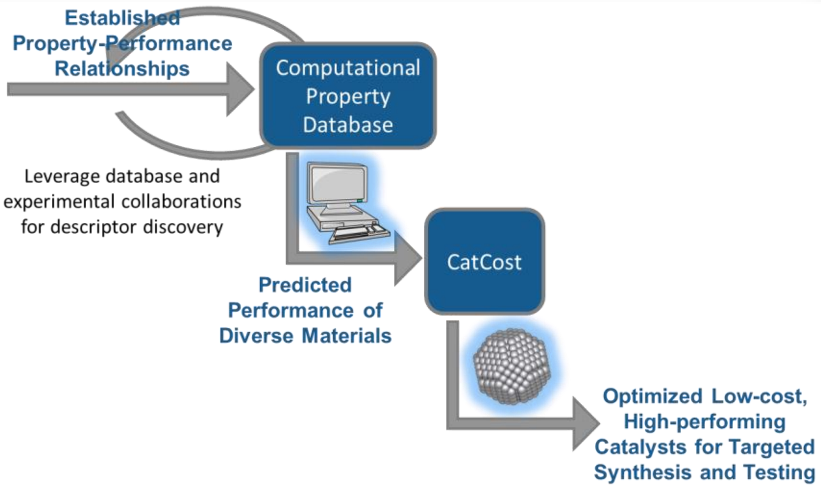
Targeted Synthesis
Identical Catalyst
Identical Yield
52% Cost Reduction





Develop an integrated catalyst design engine

- Broad applicability
- Leverages prior investment in *CatCost* development and ongoing CCPC modeling
- Accelerates the design of optimized catalyst formulations

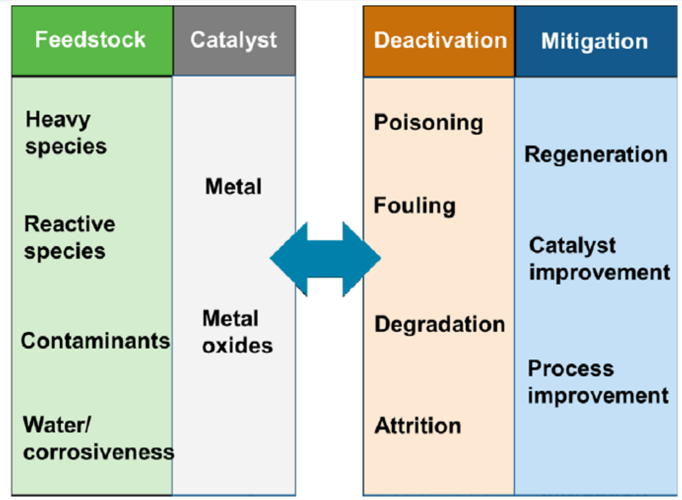


Future Work: Probing Deactivation

Leverage ChemCatBio enabling capabilities to identify deactivation modes across all core catalytic technologies

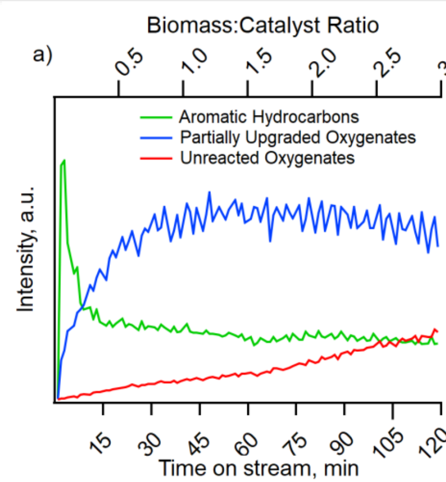
Kick-start new Catalyst Deactivation Mitigation (CDM) project

- Identify previous and ongoing efforts on catalyst deactivation/mitigation
- Establish relationships between properties of feedstock/catalyst and deactivation
- Share insight broadly with ChemCatBio teams and the research community



Evaluate deactivation and regeneration/mitigation strategies for key catalytic technologies

- All core catalytic technology projects have a milestone in FY19 focused on understanding deactivation
- Develop industrially-relevant regeneration approaches
- Work with CDM to develop mitigation strategies



Pt/TiO_2 CFP

Summary

Goal: ***Overcome catalysis challenges*** for the conversion of biomass and waste resources into fuels, chemicals, and materials by leveraging unique U.S. DOE national lab capabilities

Approach and Progress: Collaborative, early-stage R&D approach guided by TEA and stakeholder/IAB input that targets both pathway-specific and overarching catalysis challenges, ***resulting in reductions in biofuel production costs through catalysis advancements, development of tools that improve research efficiency, and industry partnerships seeking to leverage our capabilities and expertise***

Outcome: ***Accelerate the catalyst and process development cycle for bioenergy technologies***

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

Acknowledgements

ChemCatBio
Chemical Catalysis for Bioenergy

Energy Materials Network
U.S. Department of Energy

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy
Bioenergy Technologies Office

Steering Committee

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Kinga Unocic (ORNL)
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Huamin Wang (PNNL)

BETO

Nichole Fitzgerald
Kevin Craig
Jeremy Leong
Andrea Bailey

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

Thank you

ChemCatBio Team

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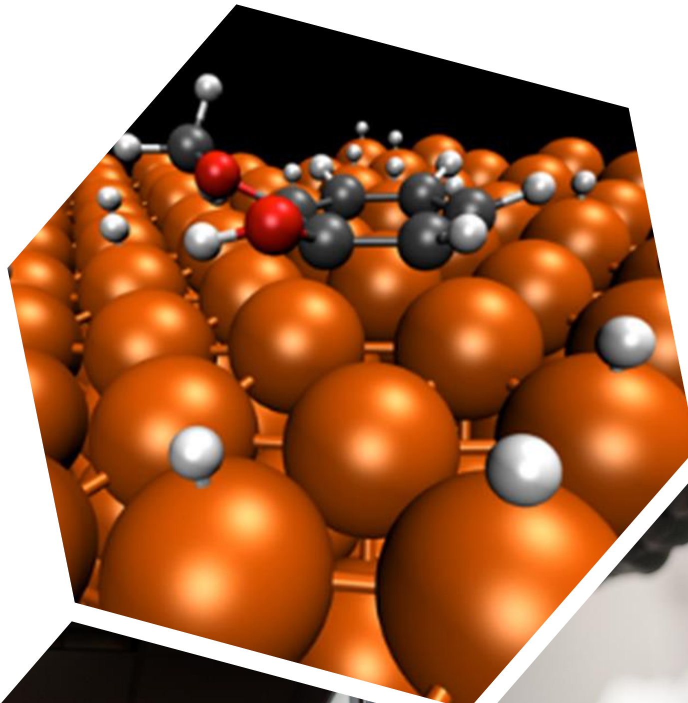
Josh Schaidle

Catalytic Upgrading

March 2019



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

Quad Chart: ChemCatBio Lead Team Support

Timeline

- Project start date: October 1st, 2016
- Project end date: September 30th, 2019
- Percent complete: 83%

	Total Costs Pre FY17	FY 17 Costs	FY 18 Costs	Total Planned Funding (FY 19-Project End Date)
DOE Funded	$0	$100k	$100k	$160k
Project Cost Share	N/A			

National Lab Partners: NREL: 85%; PNNL: 15%

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

Objective

Enable ChemCatBio to achieve its goal 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 Goal

By September 2019, this project will establish and coordinate meetings with the ChemCatBio industry advisory board, organize biannual face-to-face meetings in the spring by hosting symposia at the ACS National Meeting and in the fall hosted at a participating national lab site, initiate and organize a public webinar series for the consortium, and engage with other BETO consortia through joint webinars, meetings, and collaborative research.

Acronyms

- ACSC – Advanced Catalyst Synthesis and Characterization
- CCPC – Consortium for Computational Physics and Chemistry
- CDM – Catalyst Deactivation Mitigation (new start project in FY19)
- CFP – Catalytic Fast Pyrolysis
- CUBI – Catalytic Upgrading of Biochemical Intermediates
- DME – Dimethyl Ether
- FY – Fiscal Year
- GGE – Gasoline Gallon Equivalent
- IAB – Industry Advisory Board
- IDL – Indirect Liquefaction (or Gasification)
- MFSP – Minimum Fuel Selling Price
- MON – Motor Octane Number
- MSW – Municipal Solid Waste
- MYP – BETO's Multi-Year Plan
- PI – Principal Investigator
- RON – Research Octane Number
- STEM – Scanning Transmission Electron Microscopy
- TCF – DOE Technology Commercialization Fund
- TEA – Technoeconomic Analysis
- TOS – Time on Stream
- TPA – Terephthalic Acid
- XPS – X-ray Photoelectron Spectroscopy

Responses to Previous Reviewers' Comments

We greatly appreciate the reviewers' constructive feedback. We agree that the consortium has great potential to accelerate catalyst development and lead to greater technology advancements. The reviewers have adeptly identified many of the key success factors to the consortium including industry engagement, a clear value proposition that does not compete with existing entities in the catalyst development ecosystem, focusing on fundamentals that enable deployment, and fostering synergies between the core and enabling projects. We will use this excellent feedback to guide our path forward.

We agree with the reviewers that forming the industrial advisory board (IAB) and engaging industry are keys to the success of the consortium. We are actively working on forming the IAB and have scheduled our first stakeholder listening day for June 9th, to be held in conjunction with the North American Catalysis Society meeting in Denver, CO. We just finished drafting an IAB charter and have a list of potential members that we will be reaching out to within the next couple of months. These potential members have diverse backgrounds and experience and can provide technical guidance, insights into industrial relevance, 'big picture' perspectives, and policy implications. We plan to use our first stakeholder listening day in June to shape our value proposition for the consortium and to ensure that we are not directly competing with industry. We appreciate the guidance to focus on the fundamentals (i.e., characterization, mechanisms, modeling) and leave the commercial catalyst formulation to industry. We apologize if our use of the word "deployment" was misleading. We should have chosen a different phrase. We do not intend to be taking catalysts to market or trying to produce finished formulations. We meant that one capability of our consortium is catalyst evaluation at the pilot scale using our in-house systems, which saves money and reduces risk for industrial partners, thus enabling commercial deployment.

Even though this consortium is still in its infancy, we have already identified specific synergies, and we expect that these synergies will grow as the consortium matures. Experience from the Consortium for Computational Physics and Chemistry suggests it takes over three years before such a complex team is fully integrated and synergies are being turned into success stories. We are leveraging their experience to hopefully reach that point sooner for ChemCatBio. We expect to demonstrate significant successes in the coming years that would not have been possible without the consortium structure and agree with the reviewers that this is a key success factor of the consortium.

We thank the reviewers for their suggestion to evaluate ideas from outside the labs in the patent and open literature and reach out specifically to those groups. We also appreciate the suggestion to evaluate more industry standard catalyst materials to compare to catalysts under development within the consortium. We will pursue both of these approaches moving forward.

Go/No-Go Review Highlights (March 2018)

- **ACSC:** Demonstrated the complete catalyst development cycle for IDL and developed/incorporated new capabilities (e.g., operando XPS and STEM) to address catalyst deactivation
- **IDL:** Demonstrated increased distillate yield for all conversion pathways resulting in MFSP reductions; yield improvements achieved by modifying catalyst composition/functionality to improve carbon selectivity to critical olefinic intermediates
- **CUBI:** Generated sufficient sample quantify for fuel analysis from three process routes (carboxylic acids, 2,3-butanediol, and furfurals); >80% of the fuel generated from all three routes was suitable for blending with diesel and/or jet
- **CFP**: Demonstrated that ex-situ fixed-bed CFP is a viable option for meeting out-year cost targets (i.e., \$3.0/GGE by 2022) and identified a route and associated technical targets to achieve \$2.5/GGE by 2030

Publications, Patents, Presentations, Awards, and Commercialization

Publications:

- ChemCatBio has published over 100 peer reviewed manuscripts in the last 3 years

Presentations:

- J. Schaidle, “The Chemical Catalysis for Bioenergy Consortium: Enabling Production of Biofuels and Bioproducts through Catalysis”, Advanced Bioeconomy Leadership Conference Next 2017. San Francisco, CA. October 17^{th}, 2017. (Invited Talk)
- Inaugural multi-day symposium hosted at the ACS National Meeting in New Orleans in March 2018 (symposium continuing in 2019)
- Workshop and tutorial for the CatCost tool held at the AICHE annual meeting in Pittsburgh PA in October 2018
- Hosted 5 public webinars (slides and recordings posted to the ChemCatBio website)
  - Topics: Consortium Overview, Upgrading of Indirect Liquefaction Intermediates, Accelerating the Catalyst Development Cycle, CatCost Tutorial, and Computational Modeling
- Numerous presentations from PI’s and Co-PI’s at national and international conferences

Publications, Patents, Presentations, Awards, and Commercialization

Patents/Commercialization:

- Multiple technologies/materials developed within ChemCatBio are available for licensing including ethanol conversion to butadiene (PNNL), ethanol conversion to jet fuel (ORNL), dimethyl ether conversion to high-octane gasoline (NREL), and transition metal phosphide/carbide nanoparticle formulations and methods of making (NREL)

Awards:

- CatCost being nominated for R&D100 Award