

U.S. DEPARTMENT OF
ENERGY

Office of
ENERGY EFFICIENCY &
RENEWABLE ENERGY

Bioenergy Technologies Office 2021 Peer Review

Catalytic Upgrading Session

Trevor Smith and Sonia Hammache, March 9 – March 12, 2021



Peer Review Agenda

DAY 2 - TUESDAY, MARCH 9, 2021 PARALLEL TECHNOLOGY AREA PROJECT REVIEW SESSIONS

Start Time EST	End Time EST	Presentation Topic	Moderator
		Gather, Tech Check, Networking Questions - 30 Min Ahead of Each Session	BETO Point of Contact (POC)
11:00 a.m.	2:35 p.m.	Advanced Algal Systems	Christy Sterner
10:45 a.m.	2:40 p.m.	Feedstock Technologies	Mark Elless
10:30 a.m.	5:10 p.m.	Biochemical Conversion and Lignin Utilization	Ian Rowe
10:20 a.m.	3:30 p.m.	Performance-Advantaged Bioproducts, Bioprocessing Separations, and Plastics	Gayle Bentley
10:00 a.m.	2:10 p.m.	Catalytic Upgrading	Trevor Smith
10:15 a.m.	4:45 p.m.	Agile BioFoundry Consortium	Jay Fitzgerald
9:45 a.m.	4:20 p.m.	Organic Waste	Beau Hoffman
11:00 a.m.	3:05 p.m.	Data, Modeling, and Analysis	Alicia Lindauer

Catalytic Upgrading Review Panel

Name	Affiliation	Previous Peer Review Experience
Dr. Jesse Bond	Syracuse University	2019 Panel
Dr. Terry Mazanec	Independent Consultant (prior Velocys, BP)	New This Year
Dr. Cory Phillips	Phillips 66	2019 Panel
Dr. Jeffrey Scheibel	Independent Consultant (prior Procter & Gamble)	2017 Panel and 2019 BC and PABP Panels
Dr. Qing Shao	University of Kentucky	New This Year



Conversion Program - Catalytic Upgrading Team



Kevin Craig
Conversion R&D
Program Manager



Trevor Smith
Technology Manager



Sonia Hammache
Technology Manager



**Nichole Fitzgerald - Feedstocks
Technologies Program Manager**



**Andrea Bailey - A&S
Technology Manager**



Jesse Glover
Session Coordinator,
Project Support



Ben Simon
Project Support

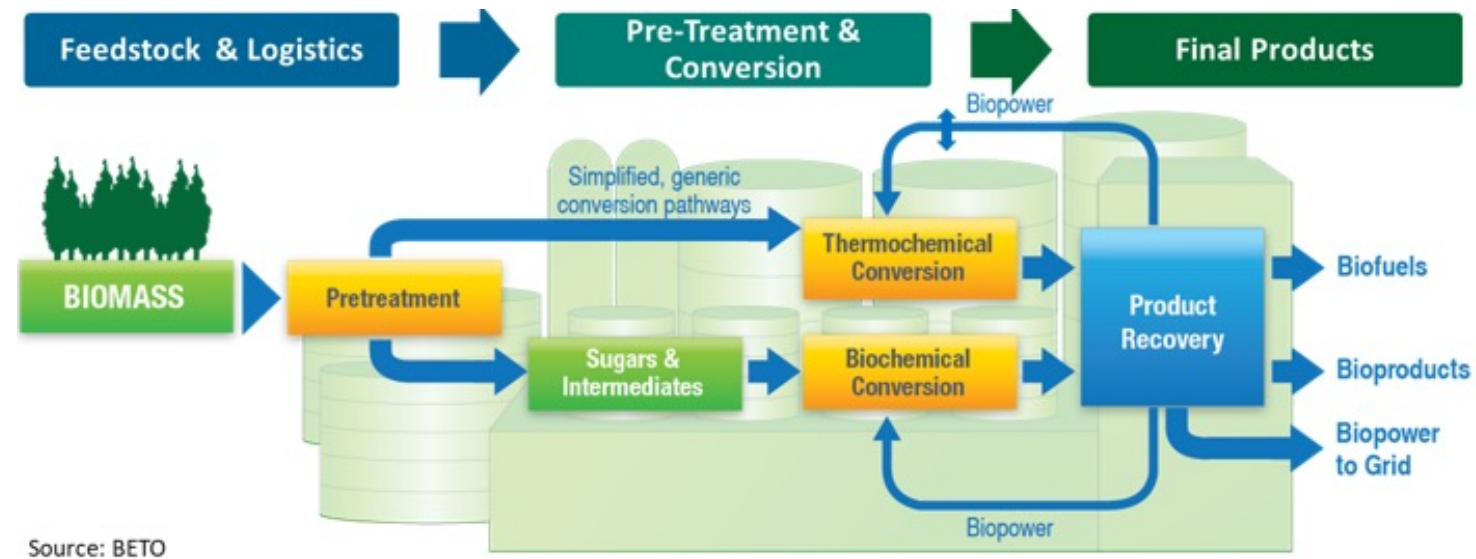
**Thank you to
former team
members!**



G. Jeremy Leong
*no longer BETO

Conversion R&D Program – Goals, Approach, Targets

- **Conversion R&D Goal:** *Develop efficient and economical technologies to convert biomass and waste feedstocks into energy-dense liquid transportation fuels, bioproducts, chemical intermediates, and biopower*
- **Conversion Approach:** *Exploring a variety of conversion technologies that can be combined into pathways from feedstocks to products*
- **Performance Target:** *By 2021, complete the research necessary to enable an integrated technology pathway verification at engineering scale in 2022 of a process that yields a mature modeled MFSP of \$3/GGE or less for production of a hydrocarbon biofuel/coproduct, with a minimum 60% reduction in GHG emissions relative to currently predominant fuel.*



Catalytic Upgrading – Key Challenges and R&D Needs

- Achieving R&D goals within pathways utilizing catalytic technologies will require:
 - Decreasing the time and cost to develop novel, industrially relevant catalysts
 - Increasing yields from catalytic processes
 - Improving catalyst lifetimes
 - Reducing risks associated with process scale up
 - Leveraging a multiscale computational framework to accelerate technology development
 - Analytical methods development

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

Catalytic Technology Area – Agenda Overview

Time	Topic
Tuesday	High temperature Catalytic Upgrading
Wednesday	Low temperature Catalytic Upgrading, Electro-catalytic upgrading, Enabling Technologies
Thursday Morning	Enabling Technologies
Thursday Afternoon	Directed Funding Awards (DFA)
Friday	Funding Opportunity Announcements (FOA) Projects

- **Annual Operating Plan (AOP) Projects**
 - Annual cycle for targeted proposals from our National Lab partners
 - Only National Labs can compete for this funding
 - ALL Chemical Catalysis for Bioenergy (ChemCatBio) consortium presentations fall under the AOP category
- **Funding Opportunity Announcements (FOA) Projects**
 - Topic-specific proposals from external applicants to support advancement of BETO goals
 - Typically, open to all (industry, academia, national labs*)
 - Required minimum recipient provided cost share


Historical Context for an Energy Materials Network

- Presidential initiative from 2011- Materials Genome Initiative (MGI)
- Addresses concerns that “the time it takes to move a newly discovered advanced material from the laboratory to the commercial market-place remains far too long.”
- Areas include Materials for National Security, Materials for Human Health and Welfare, Materials for **Clean Energy Systems**, etc.

EXECUTIVE OFFICE OF THE PRESIDENT
NATIONAL SCIENCE AND TECHNOLOGY COUNCIL
WASHINGTON, D.C. 20502

June 24, 2011

Dear Colleague:

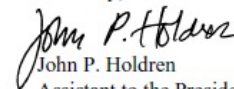


In much the same way that silicon in the 1970s led to the modern information technology industry, the development of advanced materials will fuel many of the emerging industries that will address challenges in energy, national security, healthcare, and other areas. Yet the time it takes to move a newly discovered advanced material from the laboratory to the commercial market place remains far too long. Accelerating this process could significantly improve U.S. global competitiveness and ensure that the Nation remains at the forefront of the advanced materials marketplace. This *Materials Genome Initiative for Global Competitiveness* aims to reduce development time by providing the infrastructure and training that American innovators need to discover, develop, manufacture, and deploy advanced materials in a more expeditious and economical way.

Prepared by an *ad hoc* group of the National Science and Technology Council, this initiative proposes a new national infrastructure for data sharing and analysis that will provide a greatly enhanced knowledgebase to scientists and engineers designing new materials. This effort will foster enhanced computational capabilities, data management, and an integrated engineering approach for materials deployment to better leverage and complement existing Federal investments.

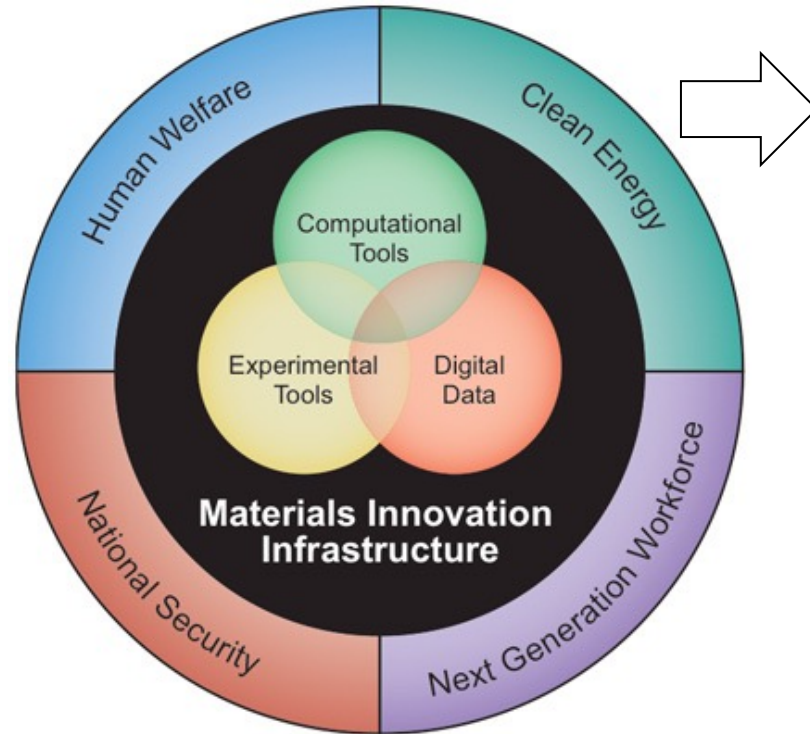
The success of this initiative will require a sustained effort from the private sector, universities, and the Federal Government. I look forward to working with you to make this vision a reality.

Sincerely,



John P. Holdren
Assistant to the President for Science and Technology
Director, Office of Science and Technology Policy

2016: EERE develops EMN in response to MGI



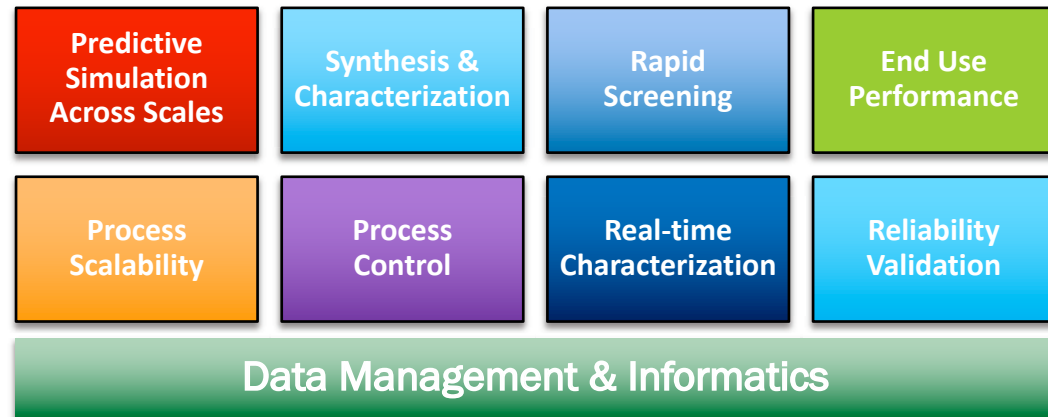
MGI - Framework



Energy Materials Network

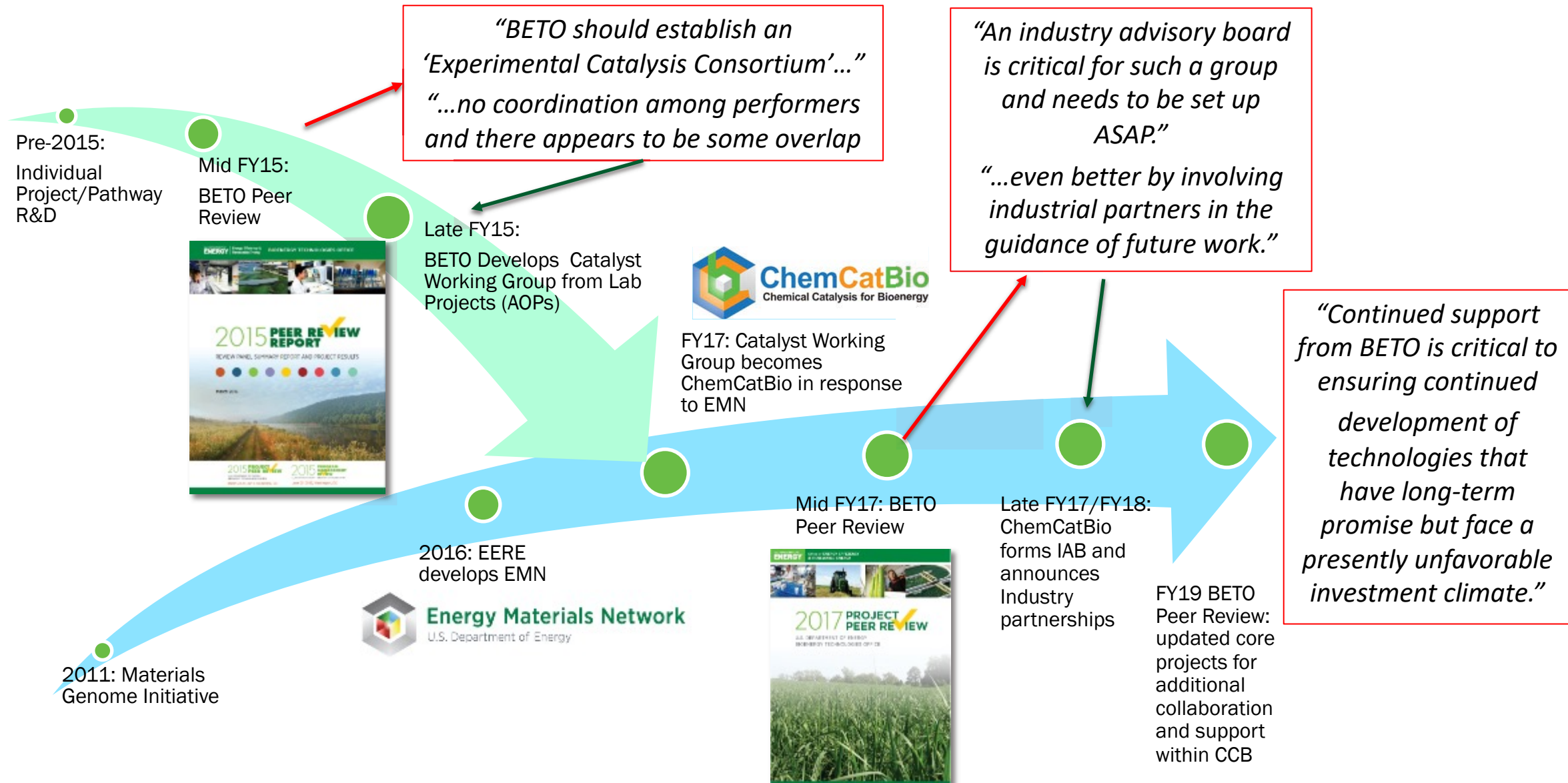
U.S. Department of Energy

Coordinated resource network with a suite of capabilities for advanced materials R&D



New Material Innovations for Clean Energy 2X Faster and 2X Cheaper

Merging Responses at Different Levels Created ChemCatBio



Fast Forward to 2021 – ChemCatBio

- **Consortium Continues to Evolve**
 - Reorganized Catalytic Technologies based on peer review and industry feedback
 - Improved Coordination; joint milestones between technologies and enabling projects
 - Expanded collaborations with other BETO consortia (FCIC, Separations, Co-Optima)
- **Focus on Industry Relationships**
 - Industry Advisory Board (IAB) interactions
 - Launched additional Directed Funding Opportunities
 - Continued outreach to encourage partnerships
 - www.chemcatbio.org, webinar series, newsletter, ACS sessions
- **Upcoming Decisions (2021-2022)**
 - New ideas based on industry feedback
 - Critical decisions related to research targets
 - Welcome feedback on future directions



ChemCatBio Projects – FY21

Integrated and collaborative portfolio of catalytic technologies and enabling capabilities

Catalytic Technologies

Catalytic Upgrading of Biochemical Intermediates

(NREL, PNNL, ORNL, LANL)

Upgrading of C1 Building Blocks
(NREL)

Upgrading of C2 Intermediates
(PNNL, ORNL)

Catalytic Fast Pyrolysis
(NREL, PNNL)

Electrocatalytic CO₂ Utilization
(NREL, will present not scored here)

Enabling Capabilities

Advanced Catalyst Synthesis and Characterization

(NREL, ANL, ORNL)

Consortium for Computational Physics and Chemistry

(ORNL, NREL, PNNL, ANL, NETL)

Catalyst Deactivation Mitigation for Biomass Conversion
(PNNL)

Industry Partnerships (Phase II Directed Funding)

Opus12 (NREL)

Visolis (PNNL)

Sironix (LANL)

*CCPC led Directed Funding:
3 new industry partnerships
starting in early 2021*

Cross-Cutting Support

ChemCatBio Lead Team Support (NREL)

ChemCatBio DataHUB (NREL)

Additional Conversion AOP Projects

- **Analytical Development and Standardization for Biomass-Derived Thermochemical Liquids (NREL, PNNL, ORNL)**
 - Enabling projects supporting industry needs
- **Enabling Complex Feedstock for Biopower Combustion and Autothermal Pyrolysis (ORNL, NREL, NETL, with industry partners)**
 - FY18 lab call to address Congressional budgetary language for “early-stage research and development projects to develop innovations in the use of biomass, municipally-derived biosolids, and sorted municipal solid waste **to improve the economic potential of biopower production and use in the United States.**”
 - Topic Area 2: Modifications to Consortium for Computational Physics and Chemistry (CCPC) Reactor Models



Projects from Funding Opportunity Announcements

- **FY15 and FY17 Biomass Research and Development Initiative (BRDI) – OSU and UT**
 - Joint Effort between the USDA and DOE, funding supports the development of a biomass-based industry in the United States. Technical areas include: Feedstocks development, **Biofuels and biobased products development**, and Biofuels development analysis.
- **FY18 BioEnergy Engineering for Products Synthesis (BEEPS) - USF and NCSU**
 - **Better utilization of waste streams** (e.g. lignin, CO₂, and biosolids), improving organic and inorganic catalysts to increase conversion efficiency and decrease costs for lignocellulosic biomass conversion, and creating high-value performance-advantaged bioproducts that can improve viability of fuel production from biomass and waste feedstocks.
 - Topic Area 1 - **ChemCatBio collaborations aimed at tackling fundamental challenges in catalysis** - catalyst characterization, catalyst development and R&D for producing engineering-relevant/technical catalysts. CCB National Laboratory partner required.
 - Topic Area 2 - **Novel alternatives to anaerobic digestion** that have the potential to compete economically with feeds of one dry ton/day or less. Alternatives with potential for direct production of higher value products from **wet waste feedstocks**.



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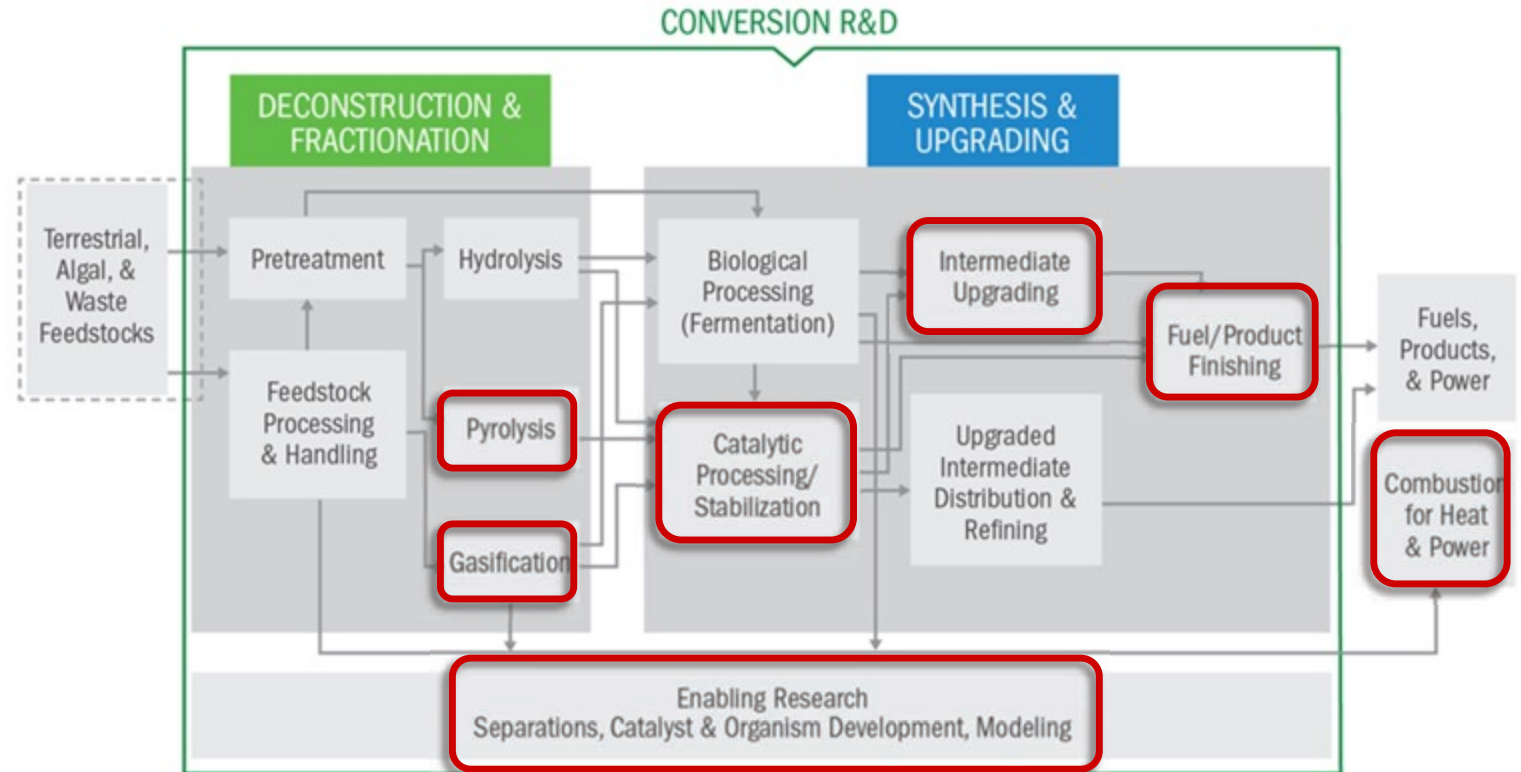


Budget Breakdown – Catalytic Upgrading

Type	FY20 - FY22
ChemCatBio AOPs	\$34.78MM
ChemCatBio Industry DFAs	(Phase I and II): \$3.93MM
FOA Projects	(all Pre-FY20): \$7.21MM
TOTAL Session	\$45.92MM

FOA Project breakdown:

- Ohio State University: \$1.5MM
- University of South Florida: \$1.84MM (\$600K to NREL)
- University of Tennessee: \$1.4MM
- North Carolina State University: \$2.47MM (\$1.225MM to NREL)



Catalytic Upgrading - Recent Successes

- 3 ChemCatBio technologies licensed by industry
 - Ethanol to jet fuel
 - Dimethyl ether to high-octane gasoline
 - Atomic Layer Deposition
- Industry leveraging unique capabilities (CCB, CCPC DFAs)
 - R&D100 Special Recognition in Green Tech (Sironix)
 - New industry partners Catalyx, Pyran and Forest Concepts leveraging modeling for scale up plans
- Accelerating catalyst-process development cycle through publicly available tools:
 - The CatCost™ Tool continues to expand, showing high utilization rates by researchers
<https://catcost.chemcatbio.org/>
 - Data Hub project released the Catalyst Property Database: A centralized, searchable compilation of published density functional theory adsorption data:
<https://cpd.chemcatbio.org/>
- Expanded research pathways with waste feedstocks and new co-products (FOA projects)

Housekeeping - Review Process

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Presentations and Review Structure

- Project Overview - provides context and history
 - Some Catalytic Technologies within CCB will present additional Techno-Economic Analyses info for additional context
- Review Criteria Sections (equal weighting)
 - Management
 - Approach
 - Impact
 - Progress and Outcomes
- Summary
- Additional Support Slides (list of publications, patents, etc.)

Detailed Catalytic Upgrading Agenda

Day 2 - TUESDAY, MARCH 9, 2021

Start Time EST	End Time EST	CATALYTIC UPGRADING		
		Presentation	Organization	Presenter
9:30 AM	10:00 AM	GATHER, TECH CHECK, NETWORKING QUESTIONS - 30 MIN AHEAD OF EACH SESSION		
10:00 AM	2:10 PM	Catalytic Upgrading	<i>Conversion Program</i>	<i>Trevor Smith and Sonia Hammache</i>
10:00 AM	10:30 AM	Catalytic Upgrading Technology Area Introduction	<i>BETO</i>	<i>Trevor Smith and Sonia Hammache</i>
10:30 AM	11:00 AM	Overview of Chemical Catalysis for Bioenergy Consortium	<i>NREL</i>	<i>Josh Schaidle</i>
11:00 AM	11:35 AM	ChemCatBio Data Hub	<i>NREL</i>	<i>Kurt Van Allsburg</i>
11:35 AM	11:45 AM	BREAK		
11:45 AM	12:20 PM	Thermochemical Platform Analysis	<i>NREL</i>	<i>Abhijit Dutta</i>
12:20 PM	12:50 PM	LUNCH (REVIEWER LUNCH TOGETHER, PUBLIC ON THEIR OWN)		
12:50 PM	1:25 PM	Upgrading of C1 Building Blocks	<i>NREL</i>	<i>Dan Ruddy</i>
1:25 PM	1:35 PM	BREAK		
1:35 PM	2:10 PM	Catalytic Upgrading of Pyrolysis Products	<i>NREL</i>	<i>Michael Griffin</i>
2:10 PM	2:40 PM	Comment Review/Daily Debrief	<i>Reviewers</i>	



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Detailed Catalytic Upgrading Agenda - Day 3

Day 3 – WEDNESDAY, MARCH 10, 2021				
9:30 AM	10:00 AM	GATHER, TECH CHECK, NETWORKING QUESTIONS - 30 MIN AHEAD OF EACH SESSION		
10:00 AM	2:00 PM	Catalytic Upgrading	<i>Conversion Program</i>	<i>Trevor Smith and Sonia Hammache</i>
10:00 AM	11:05 AM	Catalytic Upgrading of Biochemical Intermediates	<i>NREL/PNNL/ORNL/LANL</i>	<i>Richard Elander - NREL</i>
11:05 AM	11:10 AM	BREAK		
11:10 AM	11:50 AM	Upgrading of C2 Intermediates	<i>PNNL</i>	<i>Rob Dagle</i>
11:50 AM	12:25 PM	Liquid Fuels via Upgrading of Indirect Liquifaction Intermediates	<i>ORNL</i>	<i>Zhenglong Li</i>
12:25 PM	12:55 PM	LUNCH (REVIEWER LUNCH TOGETHER, PUBLIC ON THEIR OWN)		
12:55 PM	1:15 PM	Electrocatalytic CO2 Utilization	<i>NREL</i>	<i>Jack Ferrell</i>
1:15 PM	1:25 PM	BREAK		
1:25 PM	2:00 PM	Catalyst Deactivation Mitigation for Biomass Conversion	<i>PNNL</i>	<i>Huamin Wang</i>
2:00 PM	2:30 PM	Reviewer Wrap Up and Debrief	<i>Reviewers</i>	

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Detailed Catalytic Upgrading Agenda - Day 4

Day 4 - THURSDAY, MARCH 11, 2021				
Start Time EST	End Time EST	CATALYTIC UPGRADING		
		Presentation	Organization	Presenter
9:30 AM	10:00 AM	GATHER, TECH CHECK, NETWORKING QUESTIONS - 30 MIN AHEAD OF EACH SESSION		
10:00 AM	3:25 PM	Catalytic Upgrading	<i>Conversion Program</i>	<i>Trevor Smith and Sonia Hammache</i>
10:00 AM	10:50 AM	Consortium for Computational Physics and Chemistry	ORNL/NREL/PNNL/ANL/NETL	Jim Parks II - ORNL
10:50 AM	11:35 AM	Advanced Catalyst Synthesis and Characterization	NREL/ANL/ORNL	Susan Habas - NREL
11:35 AM	11:45 AM	BREAK		
11:45 AM	12:20 PM	Analytical Development and Standardization for Biomass-derived Thermochemical Liquids	NREL	Jack Ferrell
12:20 PM	12:50 PM	LUNCH (REVIEWER LUNCH TOGETHER, PUBLIC ON THEIR OWN)		
12:50 PM	12:55 PM	Directed Funding Awards Introduction	BETO	Sonia Hammache
12:55 PM	1:30 PM	Low Pressure Hydrogenolysis Catalysts for Bioproduct Upgrading w/Visolis	PNNL/Visolis	Karthi Ramasamy - PNNL
1:30 PM	1:40 PM	BREAK		
1:40 PM	2:15 PM	Catalytic Process Intensification of Bio-Renewable Surfactants Platform w/Sironix	LANL/Sironix	Cameron Moore - LANL
2:15 PM	2:50 PM	Catalyst Development for Selective Electrochemical Reduction of CO2 to High-value Chemical Precursors w/Opus-12	NREL/Opus-12	Frederick Baddour - NREL
2:50 PM	3:25 PM	Enabling Complex Biomass Feedstock for Biopower Combustion and Autothermal Pyrolysis	ORNL/NREL/NETL	Jim Parks II - ORNL
3:25 PM	3:55 PM	Reviewer Wrap Up and Debrief	<i>Reviewers</i>	

Directed Funding Awards (DFA) - CRADA Partnerships

Phase I – Late FY18-2020

Company	Labs	CCB Capabilities	Product
GEVO (mixed oxide)	NREL, ANL, ORNL	Characterization	C ₃ -C ₄ olefins
Vertimass	NREL, ANL, ORNL	Characterization	Hydrocarbon fuels
Lanzatech (Terephthalic Acid)	PNNL	Synthesis, Characterization, Evaluation, Modeling	Terephthalic acid
GEVO (Tactical Aviation Fuels)	LANL	Synthesis, Characterization, Evaluation, Modeling	Cyclobutanes
ALD Nanosolutions and JM	NREL	Synthesis, Characterization, Evaluation, Modeling	Hydrocarbons
Lanzatech (Fuel Fractions)	PNNL	Evaluation, Modeling	Jet fuel
<i>Visolis</i>	NREL	Synthesis, Evaluation	Diols
<i>Opus-12</i>	NREL	Synthesis, Characterization, Evaluation	Alcohols
<i>Sironix</i>	LANL	Synthesis, Characterization, Evaluation, Modeling	Oleo-furan surfactants



Phase II - FY20



Directed Funding Awards (DFA) - CRADA Partnerships: Phase 2

Directed Funding Awards	Phase 1	Phase 2
<p>Visolis and PNNL: Low Pressure Hydrogenolysis Catalysts for Bioproduct Upgrading</p>	<ul style="list-style-type: none"> Catalyst identification and optimization Catalyst stability 100 hrs. 	<ul style="list-style-type: none"> Catalyst impurity tolerance Extruded catalyst stability 500 hrs.
<p>Sironix and LANL: Catalytic Process Intensification of Bio-Renewable Surfactants Platform</p>	<ul style="list-style-type: none"> Selective reduction & furan coupling catalysts Optimize catalyst for scale up 	<ul style="list-style-type: none"> Alternative coupling catalysts for new tail options Develop and test catalysts for furan-tail coupling approaches
<p>Opus 12 and NREL: Catalyst Development for Selective Electrochemical Reduction of CO₂ to High-value Chemical Precursors</p>	<ul style="list-style-type: none"> Cathode catalyst development Reactor integration and catalytic evaluation 	<ul style="list-style-type: none"> Scale up of cathode catalyst



Additional Conversion AOP Project

- **Enabling Complex Feedstock for Biopower Combustion and Autothermal Pyrolysis (ORNL, NREL, NETL, with industry partners)**
 - FY18 lab call to address Congressional budgetary language for “early-stage research and development projects to develop innovations in the use of biomass, municipally-derived biosolids, and sorted municipal solid waste **to improve the economic potential of biopower production and use in the United States.**“
 - Topic Area 2: Modifications to Consortium for Computational Physics and Chemistry (CCPC) Reactor Models
- **Project began in mid 2019 (poster review at 2019 BETO Peer Review)**



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10:00 AM	10:05 AM	Introduction to Catalytic Upgrading Projects from FOAs	<i>BETO</i>	<i>Trevor Smith</i>
10:05 AM	10:40 AM	Biomass Gasification for Chemicals Production Using Chemical Looping Techniques	<i>The Ohio State University</i>	<i>Andrew Tong</i>
10:40 AM	11:15 AM	Intensified Biogas Conversion to Value-Added Fuels and Chemicals	<i>University of South Florida</i>	<i>John Kuhn</i>
11:15 AM	11:25 AM	BREAK		
11:25 AM	12:00 PM	Condensed Phase Catalysis Technology for Fuels and Carbon Products	<i>University of Tennessee - Knoxville</i>	<i>David Harper</i>
12:00 PM	12:35 PM	Catalytic Upgrading of Carbohydrates in Waste Streams to Hydrocarbons	<i>North Carolina State University</i>	<i>Sunkyu Park</i>
12:35 PM	1:05 PM	LUNCH (REVIEWER LUNCH TOGETHER, PUBLIC ON THEIR OWN)		
1:05 PM	2:05 PM	Reviewer Wrap Up and Debrief	<i>Reviewers</i>	

Projects from Funding Opportunity Announcements

- **FY15 and FY17 Biomass Research and Development Initiative (BRDI) – OSU and UT**
 - Joint Effort between the USDA and DOE, funding supports the development of a biomass-based industry in the United States. Technical areas include: Feedstocks development, **Biofuels and biobased products development**, and Biofuels development analysis.
- **FY18 BioEnergy Engineering for Products Synthesis (BEEPS) - USF and NCSU**
 - **Better utilization of waste streams** (e.g. lignin, CO₂, and biosolids), improving organic and inorganic catalysts to increase conversion efficiency and decrease costs for lignocellulosic biomass conversion, and creating high-value performance-advantaged bioproducts that can improve viability of fuel production from biomass and waste feedstocks.
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