

# 2019 PROJECT JEW

U.S. DEPARTMENT OF ENERGY BIOENERGY TECHNOLOGIES OFFICE

## **Conversion Technologies Research & Development**

**Kevin Craig** 

Program Manager, Conversion R&D

March 4<sup>th</sup>, 2019

- Conversion Team Introduction
- Conversion Goals and Approaches
- Portfolio Structure, Challenges, and Budget
- FOA and Other Awards
- Accomplishments and Direction
- New and expanded R&D Areas
- Review Panel Introduction



## **Conversion R&D Team – DOE and Fellows**

#### Kevin Craig, Program Manager



## **DOE Staff**

David Babson

Jay Fitzgerald

Nichole Fitzgerald

Beau Hoffman

lan Rowe

Liz Moore\*

ORISE Fellows

Andrea Bailey

Jeremy Leong



David

lan

Jeremy



Jay



Andrea



Nichole



Beau









## **Conversion R&D Team – Support Contractors**

#### **Conversion Support Contractors**

Josh Messner - AST, Manager

Mark Philbrick – AST

Jessica Phillips – AST

Clayton Rohman – AST

Trevor Smith – AST

Seth Menter - AST

Robert Natelson – AST

Camryn Sorg – The Building People, LLC



Josh



Trevor



Robert



Camryn



Seth







Jessica



Clayton



# • **BETO Strategic Goal:** Enable use of America's abundant biomass and waste resources for advanced biofuels, bioproducts, and biopower by:

- Identifying and developing biofuel pathways and innovative end uses;
- Lowering the cost of production through increased efficiency, productivity, and yields; and
- Completing applied research and development on complex, real world systems, and integrating engineering processes for promising new advanced bioenergy technologies

while maintaining or enhancing economic, environmental, and social sustainability.



• **Conversion R&D Goal:** Develop efficient and economical biological and chemical technologies to convert biomass feedstocks into energy-dense liquid transportation fuels, such as renewable gasoline, diesel, and jet fuel, as well as bioproducts, chemical intermediates, and biopower.

#### **Approaches:**

- Enhance U.S. industrial competitiveness by reducing time-to-market, improving yields, and increasing selectivity
- Fund research that supports a diversity of biochemical, thermochemical, and hybrid conversion technologies to match the distributed, diverse, domestic resources
- Leverage biological pathway engineering science
- Develop better catalysts and organisms faster through applied science



*Price-competitive technologies for converting biomass into fuels and products* 



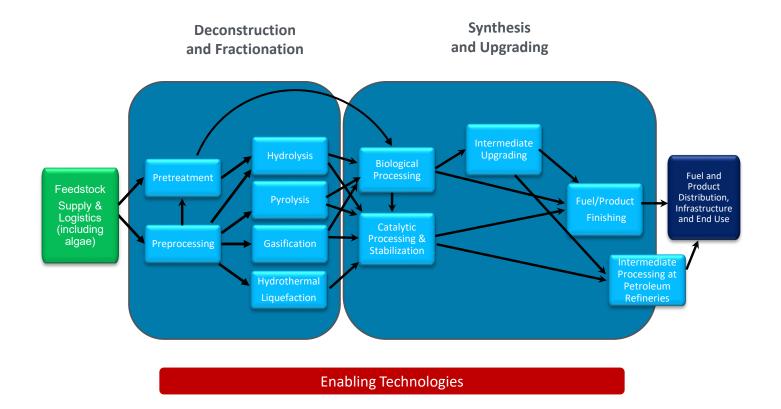


#### PORTFOLIO STRUCTURE AND BUDGET



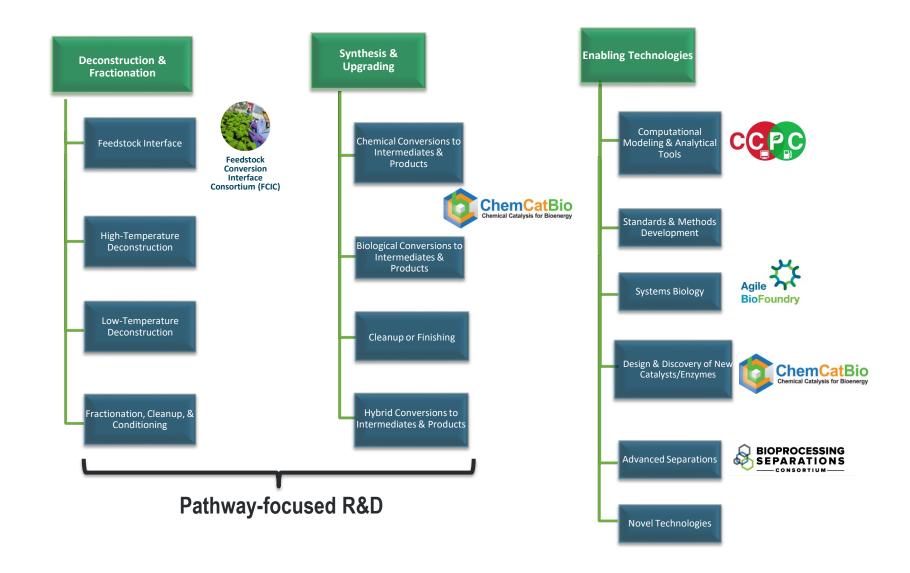


### Pathways are collections of technologies and interfaces



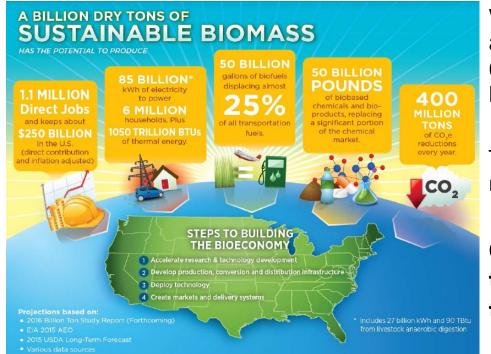


#### **Program Structure**





# The Challenge: How can BETO enable cost-competitive (<\$3/GGE) lignocellulosic biofuels in the near term (~5-10 years)?



We annually model and periodically verify 6 lignocellulosic biofuel pathways

The average MSFP at nth plant is \$3.36/GGE

Can bioproducts be the thin edge of the wedge?

"An assessment of the potential products and economic and environmental impacts resulting from a billion ton bioeconomy" Biofuels, Bioprod. Bioref. 11:110–128 (2017). Z Haq (BETO) and partners at USDA, Energetics, AST, and ANL





Molecule	Company	Cost	Time
1,3-Propanediol (PDO)	DuPont - Tate & Lyle	>>\$120M	15 years
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Artemisinin	UC Berkeley, Amyris, Sanofi	>\$50M	10 years

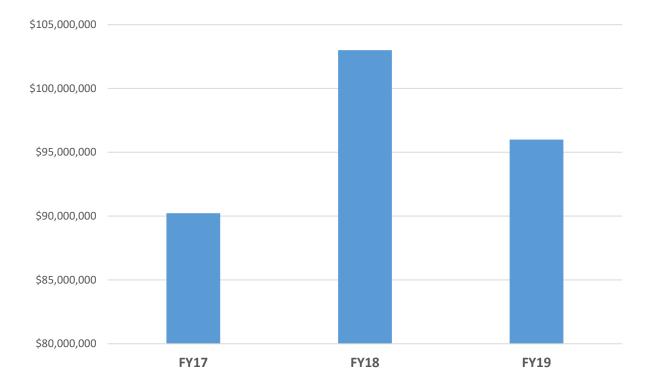
Possible savings of *billions* of dollars by reducing development time of products, reducing energy intensity and increasing carbon efficiency





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# **Total Conversion Budget by FY for the Review Period**





## **Portfolio Overview – National Lab Work FY17-FY19**

ABF	FCIC	FCIC PI Co-pr		l Methods
ССВ	Biologica Pathway:		CO2, WTE, Novel Feedstocks	Analysis + Analytical Methods
ССРС	Separations		Lignin	PABP

ABF	\$47,800,000
Analysis +	
Analytical Methods	\$14,700,000
<b>Biological Pathways</b>	\$24,500,000
ССВ	\$32,600,000
ССРС	\$13,250,000
FCIC	\$10,800,000
PABP	\$4,340,000
CO2, WTE, + Other	
Novel Feedstocks	\$15,000,000
Lignin	\$10,700,000
Separations	\$10,750,000
PDUs + Co-	
processing	\$12,500,000

\$1M

Enabling Technologies

Pathway Specific



## Portfolio Overview – Including Awarded Competitive Funds FY17-FY19

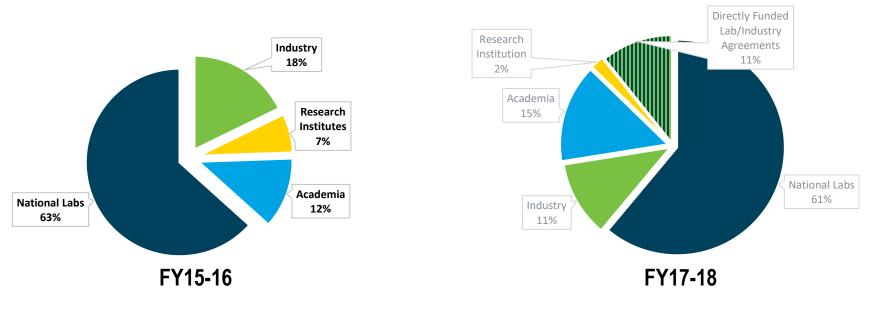
ABF	Ligniı	n	CO2, W/TE Novel		ABF Analysis + Analytical Methods Biological Pathways	\$60,300,000 \$14,700,000 \$24,500,000 \$40,400,000			
		Biologi	ral .	Feedstocks		ССВ ССРС FCIC PABP CO2, WTE, + Other	\$13,250,000 \$10,800,000 \$13,340,000		
ССВ		Pathways Analysis + Analytical Methods		Novel Feedstocks Lignin Separations PDUs + Co- processing	\$26,000,000 \$15,200,000 \$10,750,000 \$12,500,000				
		PDUs + Co- processing			РАВР	\$1M Enabli Technolo			
Separations	FCIC	1			locessing			Pathway S	pecific

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### **Portfolio Structure**

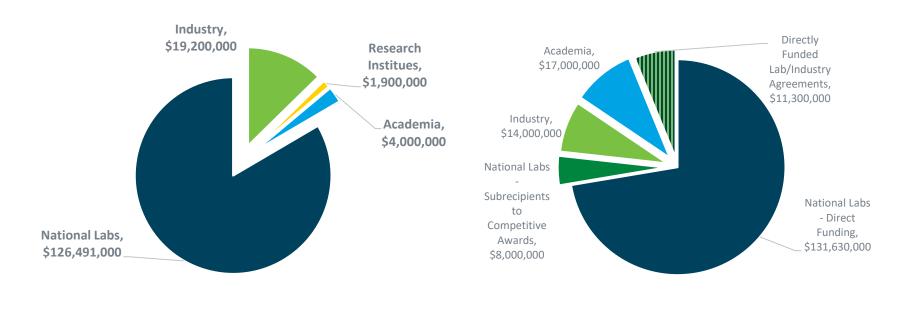
# 149 total Conversion portfolio projects to be reviewed over the next four days:

- 27 in the Biochemical Review Session
- 10 in the ABF Review Session
- 24 in the Catalysis Review Session
- 11 in the Waste to Energy (WTE) Session
- 14 in the PABP/Seps Review Session
- 11 in the Lignin Review Session
- 7 in the CO2 Review Session
- 32 in the Poster Session
- 12 in additional review sessions from other programs





#### Amount Appropriated During Review Period by Recipient Type (numbers rounded)



FY15-16

FY17-18



## **Ex-situ CFP**

1. Total Capital Investment (-15% : base : +30%)	-8.0%	16.1%
2. Feedstock Cost, \$/dry U.S. ton (60 : 80 : 120)	-7.8%	15.7%
<ol> <li>Internal Rate of Return / Discount Rate for DCFROR (5 : 10 : 15 %)</li> </ol>		
	-14.8%	15.4%
4. HGF, Capital Cost + 10% Yield Loss (No HGF : No HGF : HGF with loss)	0.0%	15.2%
5. Ex Situ Organic Liq. Yield;C Efficiency % (30;49 : 27;44 : 24;39)	-8.1%	11.6%
<ol><li>Plant Size (10,000 : 2,000 : 1,000 dry metric tonnes/day)</li></ol>	-10.0%	8.1%
<ol><li>Vapor Upgrading Catalyst Unit Cost, \$/b (3.25 : 9.75 : 19.50)</li></ol>	-6.4%	9.6%
8. Fast Py. & Ex Situ Reactor Capital (-20% : base : +40%)	-4.6%	9.2%
9. Hydroprocessing C Efficiency (94 : 94 : 88 %)	0.0%	9.0%
10. Interest Rate on Debt (4% : 8% : 12%)	-5.3%	5.6%
11. Vapor Upgrading Catalyst Replacement, %/day (1:2:4)	-2.7%	5.3%
12. Plant Life (30 : 30 : 20 years)	0.0%	4.1%
13. Ex Situ Catalyst:Biomass w/w Circulation (6 : 6 : 7)	0.0%	3.9%
14. Hot Gas Filter, HGF, Capital Cost Only (No HGF : No HGF : HGF no loss)	0.0%	3.2%
15. Hydrogen Plant Capital (-20% : base : +30%)	-2.0%	3.0%
16. Time on Stream (94% : 90% : 88%)	-2.5%	2.7%
17. Stearn & Power Plant Capital (-20% : base : +30%)	-1.5%	2.3%
18. Hydrotreating Catalyst Unit Cost, \$/lb (10 : 20 : 60)	-0.6%	2.2%
19. Hydroprocessing & Separation Capital (-20% : base : +40%)	-1.0%	2.1%
20. C Loss as Coke (vs. Gas) with Constant Organic Liquid Yield (7%: 8%: 9%)	-0.4%	1.2%
21. Wastewater Management Capital (-20% : base : +50%)	-0.4%	1.0%
22. No Vapor Heat Recovery Below Temp. (175 : 175 : 931 °F). No New Equip.	0.0%	0.9%
23. Electricty Credit Impact, No Capital Change (base : base 2.6¢ : no credit)	0.0%	0.8% Market, Finance etc.
24. Hydrocracking Catalyst Unit Cost, \$/lb (10 : 20 : 60)	-0.2%	0.7% Vapor Upgrading
25. No. of HT Reactors x %Capacity (1x100 : 1x100 : 3x50)	0.0%	0.7% Hydroprocessing
26. Heat Loss During Pyrolysis & Vapor Upgrading, % LHV Biomass (3 : 3 : 6)	0.0%	0.4% Balance of Plant
27. Hydrotreating Pressure, (1500 : 1500 : 2000 psia)	0.0%	0.1%
-25	5% 0	% 25

% Change to MFSP from the ex situ base case (\$3.31/GGE)



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25%

CCB DFA BETO Briefing – Sept 2017

Items either not directly tied to BETO R&D or influenced by progress in the bioenergy industry as a whole were eliminated

Rank	Description	Max Impact (negative)	Max Impact (positive)
1	Total Capital Investment	-8.0%	
2	Feedstock Cost \$/dry US ton	-7.8%	15.7%
3	Internal IRR	-14.8%	15.4%
4	HGF Capital Cost	-0.0%	15.2%
5	Ex-Situ Organic Liq Yield	-8.1%	11.6%
6	Plant Size	-10.0%	8.1%
7	Vapor Upgrading Catalyst Unit Cost	-6.4%	9.6%
8	Fast Py & Ex Situ Reactor Capital	-4.6%	9.2%
9	Hydroprocessing C Efficiency	-0.0%	9.0%
10	Interest Rate on Debt	-5.3%	5.6%
11	Vapor Upgrading Catalyst Replacement	-2.7%	5.3%
12	Plant Life	-0.0%	4.1%
13	Ex Situ Catalyst Biomass with Circulation	-0.0%	3.9%
14	Hot Gas Filter, Capital Cost	-0.0%	3.2%
15	Hydrogen Plant Capital	-2.0%	3.0%
16	Time on Stream	-2.5%	2.7%
17	Steam and Power Plant Capital	-1.5%	2.3%
18	Hydrotreating Catalyst Unit Cost	-0.6%	2.2%
19	Hydroprocessing and Separation Capital	-1.0%	2.1%
20	C Loss as Coke with Constant Organic Liquid Yield	-0.4%	1.2%
21	Wastewater Management Capital	-0.4%	1.0%
22	No Vapor Heat Recovery Below Temp	-0.0%	0.9%
23	Electricity Credit Impact	-0.0%	0.8%
24	Hydroprocessing Catalyst Unit Cost	-0.2%	0.7%
25	Number of HT Reactors x %Capacity	-0.0%	0.7%
26	Heat Loss During Pyrolysis Vapor Upgrading	-0.0%	0.49
27	Hydrotreating Pressure	-0.0%	0.1%



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# **Ex-situ CFP**

### **Top 10 remaining areas by current active project:**

Rank	Description	FSL Core Work (INL, ORNL)
2	Feedstock Cost \$/dry US ton	
4	HGF Capital Cost + Yield C Efficiency	Ex-Situ CFP (NREL, PNNL)
5	Ex-Situ Organic Liquid Yield	dvanced Catalyst Synthesis and
7	Vapor Upgrading Catalyst Unit Cost	
8	Fast Py & Ex Situ Reactor Capital	
9	Hydroprocessing C Efficiency	CCPC (ORNL, NREL, ANL, PNNL,
	Vapor Upgrading Catalyst	NETL)
11	Replacement	TCPDU (NREL)
	Ex Situ Catalyst Biomass with	Corrosion Studies (ORNL)
13	Circulation	- Big-Oil Standardization (NREL, PNN
15	Hydrogen Plant Capital	
16	Time on Stream	Potential Biopower Selections



# **Ex-situ CFP**

#### **Top 10 remaining areas by FY17 investment:**

Rank	Description	FY17 Investment (\$K)
	Feedstock Cost \$/dry US ton	\$1,600
4	HGF Capital Cost + Yield C Efficiency	\$4,000
5	Ex-Situ Organic Liquid Yield	\$4,750
7	Vapor Upgrading Catalyst Unit Cost	\$7,925
8	Fast Py & Ex Situ Reactor Capital	\$7,550
9	Hydroprocessing C Efficiency	\$4,750
11	Vapor Upgrading Catalyst Replacement	\$7,925
13	Ex Situ Catalyst Biomass with Circulation	\$7,925
15	Hydrogen Plant Capital	\$0
16	Time on Stream	\$7,550



## FOA and Direct Funding Opportunities







### **Bioenergy Engineering for Products Synthesis (BEEPS) FOA**

On May 5,<sup>th</sup> 2018 the U.S. Department of Energy (DOE) announced a FOA to support R&D to develop highly efficient conversion processes for improving the affordability of fuels and products from biomass and waste streams.

FOA Topic Areas:

- Topic Area 1: ChemCatBio Industrial Partnerships (CCB)
- Topic Area 2: Agile BioFoundry Industry Partnership Initiative (ABF)
- **Topic Area 3:** Performance Advantaged Bioproducts (PABP)
- Topic Area 4: Biofuels and Bioproducts from Wet Organic Waste Strean
- Topic Area 5: Rewiring Carbon Utilization (Rewiring)
- Topic Area 6: Lignin Valorization (Lignin)

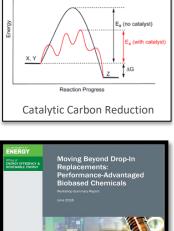
#### Funding Amount: Up to \$28,000,000



Aaile

#### *Contributions to BETO's mission:*

- R&D to increase efficiency of conversion to drive down cost of biofuels and bioproducts
- Increases industry access to capabilities to improve biofuel and bioproduct production and management through partnerships with DOE's Agile BioFoundry and ChemCatbio
- R&D in valorizing residual side streams through lignin valorization
- R&D on leveraging waste as an untapped resource with economic advantages









- Separations for Biochemical Conversion Developed in situ product recovery system to extract carboxylic acids from fermentation broth utilizing solvent/membrane systems and increased acid product concentration ~6x
- Separations for Thermochemical Conversion Developed functionalized resins and molecular sieves that exceeded FY18 target of 25% carbonyl reduction in liquid pine bio-oils
- Directed Funding Opportunity

Company w/ Labs	Feedstock	Separations	Product
Visolis w/ ANL & LBNL	Cellulosic Sugar	RW-EDI, wiped film distillation	fatty acid
Kalion w/ ORNL, ANL & NREL	Cellulosic Sugar	pervaporation, RW-EDI, nano- adsorbents	Glucaric acid
Mango Materials w/ LBNL	Biogas	Tangential Flow Filtration	PHAs from methanotrophs
DMC Biotechnologies w/ ANL	Cellulosic Sugar	Nano-adsorbents	Farnesene, liquid hydrocarbons
HelioBioSys w/ LANL & LBNL	Atmospheric CO <sub>2</sub>	Ultrasonic Separations	Extracellular polysaccharides from cyanobacterial consortium



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Company	Labs	Feedstock	Organism	Capabilities	Product
Kiverdi	NREL, LBNL, ORNL	$CO_2$ and $H_2$	Cupriavidus necator	Design: DIVA, Test: targeted –omics and biocatalyst optimization	Fatty-acid derived molecule
LanzaTech	ANL & NREL	Syngas & Waste Gas	Clostridium autoethanog enum	Learn: machine learning and deep learning	Various chemicals and fuels
Lygos	SNL, LBNL, PNNL	Cellulosic Sugar	Pichia kudriavzevii	Design: DIVA, Build, Test: Proteomics, Metabolomics, Experiment Data Depot	Organic acid
TeselaGen	LBNL, PNNL, SNL	NA	NA	Design: BOOST, BLiSS; Test: Experiment Data Depot	NA
Visolis	NREL, ORNL	Cellulosic Sugar and Waste Gas	Clostridium ljungdahlli	Build: Genetic Transformation and Tool Development	Hydroxyacid intermdiate
University of Georgia	LANL, NREL	Cellulosic Sugar	Acinetobacter baylyi ADP1	Test: Biocatalyst Optimization, High Throughput Screening	Terephthalic acid



LYGOS

teselagen BIOTECHNOLOGY

CARBON NEGATIVE MATERIALS

Franklin College of Arts and Sciences UNIVERSITY OF GEORGIA



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**Department of Microbiology** 

Company	Labs	CCB Capabilities	Product
GEVO (mixed oxide)	NREL, ANL, ORNL	Characterization	$C_3$ - $C_4$ olefins
Visolis	NREL	Synthesis, Evaluation	diols
Vertimass	NREL, ANL, ORNL	Characterization	Hydrocarbon fuels
Lanzatech (Terephthalic Acid)	PNNL	Synthesis, Characterization, Evaluation, Modeling	Terephtalic 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
Opus-12	NREL	Synthesis, Characterization, Evaluation	alcohols
Sironix Renewables	LANL	Synthesis, Characterization, Evaluation, Modeling	oleo-furan surfactants





SIRONIX

RENEWABLES

Energy Efficiency & Renewable Energy

Transformative fungible biofuels.

CARBON NEGATIVE MATE

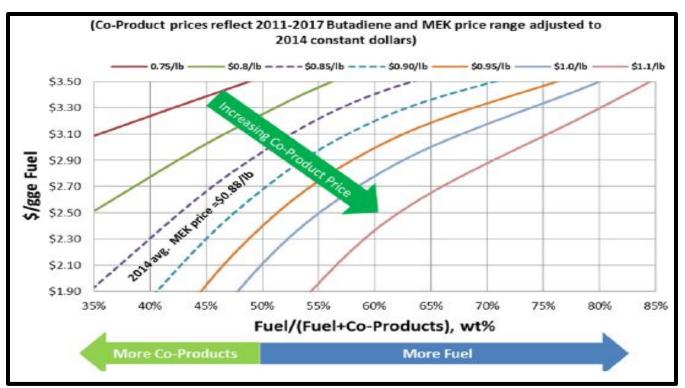
# **Accomplishments & Direction**





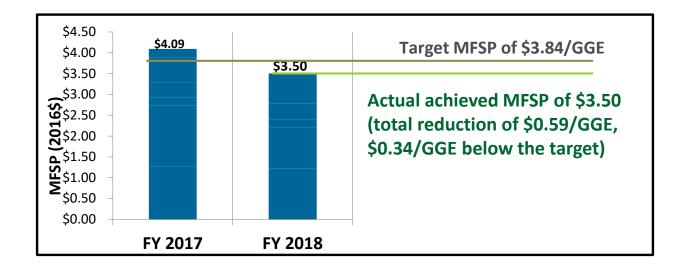
# **Achieved FY2017 Office Performance Metric**

- \$3/gge Modeled, Mature-plant Fuel Price (plant gate)
- Unanticipated problems with Fast Pyrolysis & Upgrading
- Pivoted to analysis of Lanzatech alcohol-to-jet process utilizing PNNL catalyst
  - PNNL received "Excellence in Technology Transfer Award" for this work with LanzaTech
- Highlights importance of co-products





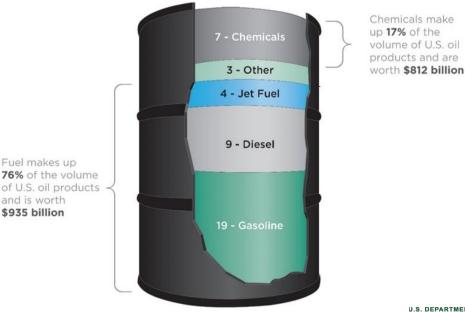
- **FY18 Office GPRA Target:** For at least one approach (e.g., in situ, ex situ, dual bed, co-processing/hydrotreating),
  - Carbon efficiency greater than 36% to fuel blendstocks. <u>Final</u>
     <u>result: 39.7%</u>
  - Reduction in the modeled MFSP by \$0.25/GGE compared to the FY17 SOT. <u>Final result: -\$0.59/GGE</u>





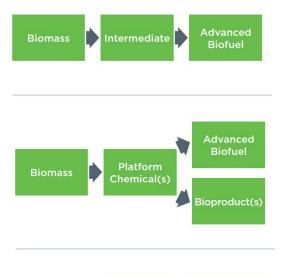
#### **Replacing the Whole Barrel – A Shift Toward Drop-ins and Bioproducts**

- Only ~40% of a barrel of crude oil is used to produce petroleum gasoline. Reducing ٠ oil dependence requires replacing diesel, jet fuel, heavy distillates, and other products.
- EERE successfully achieved modeled mature cost goals for cellulosic ethanol in 2012 and shifted its R&D to focus on hydrocarbon "drop-in" biofuels, jet fuels, and bio-based products.
- **Fuel makes up 76% of the** volume of U.S. oil products and is worth **\$935B**. ٠
- Products make up 17% of the volume of U.S. oil products and are worth **\$812B**. ٠



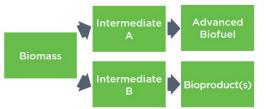






**Fuel alone**. Traditional approach which was highly successful for cellulosic ethanol

**Platform chemical**. (e.g. Vertimass EtOH to jet, levulinic acid)



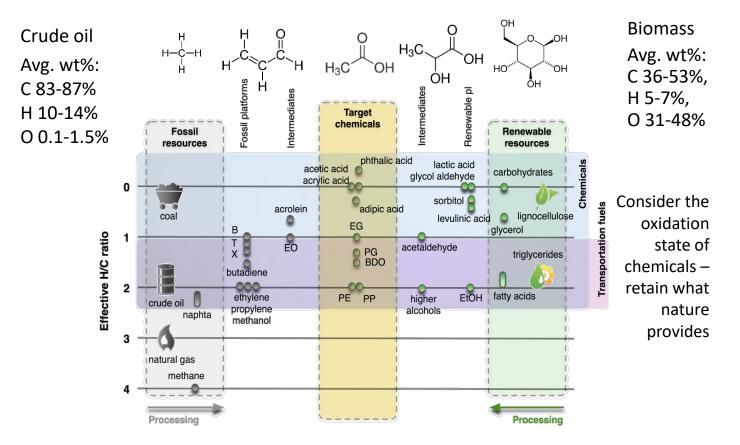


**Coproduction**. May utilize waste stream/slip stream conversion (e.g. C5 to succinic, lignin utilization, starch ethanol, etc.)

**Product alone**. De-risks upstream unit operations, builds supply infrastructure, builds investor confidence



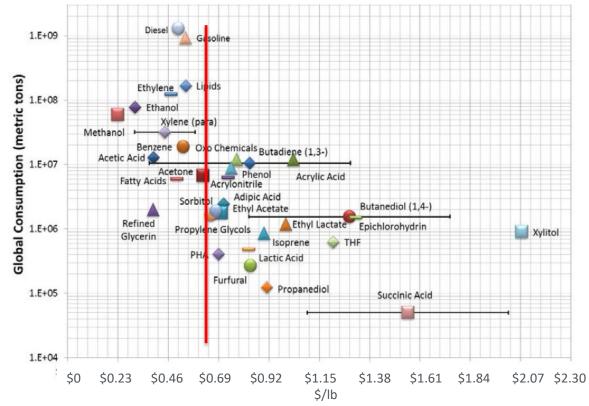
#### **Biobased products contain oxygen... like biomass**



Vennestrøm, P.N. R. et al Angew. Chem. Int. Ed. **2011**, *50*, 10502-10509 Shen, J. et al Energy Conversion and Management **2010**, *51*, 983–987



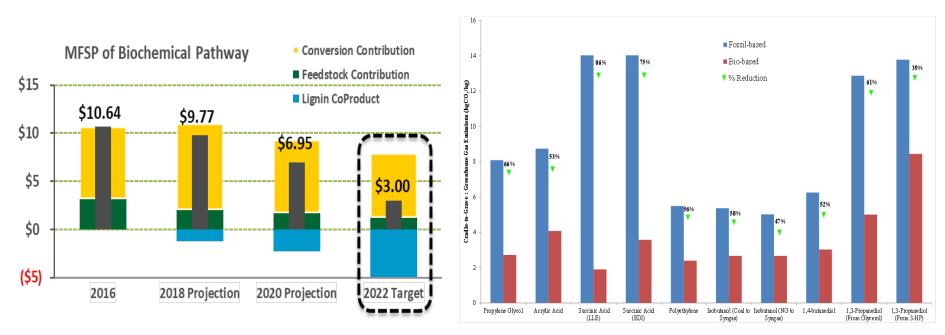
#### **Scalability of Bioproducts**



Chemicals from Biomass: A Market Assessment of Bioproducts with Near-Term Potential, Mary Biddy (NREL) and colleagues. Available at: http://www.nrel.gov/docs/fy16osti/65509.pdf



# Bioproducts uniformly showed emission reductions compared to their fossil-derived counterparts



Life-Cycle Fossil Energy Consumption and Greenhouse Gas Emissions of Bioderived Chemicals and Their Conventional Counterparts – Felix Adom, Jennifer Dunn, Jeongwoo Han, and Norm Sather.



# Consortia





#### Performance Advantaged BioProducts (PABP) Consortium

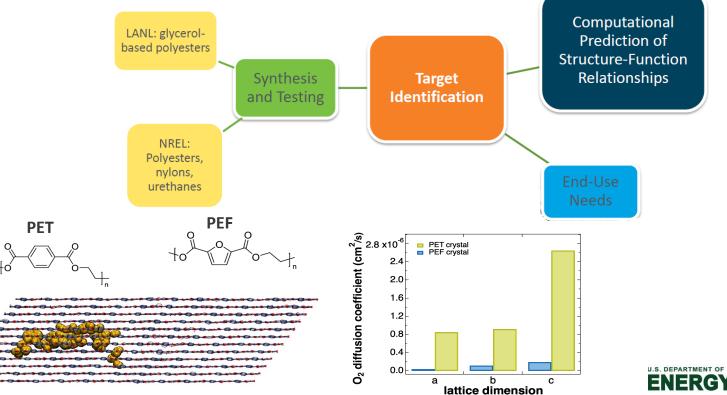
- FY18 began \$1.9M mini consortium at NREL to identify novel, performance advantaged bioproducts; FY19 introduced LANL + NREL partnership
- Three focus areas that represent workshop stakeholder concerns:
  - Computational modeling to predict how biobased compounds will behave
  - High throughput screening of biobased compounds to understand what can be easily made and what
  - End Use Needs- can we look at existing products and assess what is ripe for innovation?



Workshop in June, 2017; report PUBLISHED (check BETO website)

Energy Efficiency &

**Renewable Energy** 



#### **Agile BioFoundry**

Structure:

• Virtual consortium of 8 national laboratories

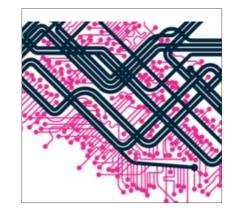
#### Goal:

- Public infrastructure to enable 50% reductions in time and cost to bring a new bio-derived chemical to market through enhance conversion efficiency Outcomes:
- 10X improvement in Design-Build-Test-Learn cycle efficiency, new host organisms, new IP and manufacturing technologies effectively translated to U.S. industry ensuring market transformation.

#### Recent Accomplishments:

- Three FY18 FOA selections awarded for Agile BioFoundry Industry Partnerships
- Constructed advanced machine learning models to improve pathway design
- 4X increase in DNA sequence validation speed (384 -> 1536 samples/week)
- PNNL/LBNL designed and built 3-hydroxpropionic acid pathway and transformed it into *Aspergillus pseudoterreus* 
  - 1st cycle demonstrated 2-3 g/L titer, and doubled the titer in 2<sup>nd</sup> cycle
- NREL/ORNL/ANL reached near-theoretical yields of muconate from glucose-fed *Pseudomonas putida* (41.3% mol/mol)
- SNL produced up to ~200 mg/L 1,8-cineole on modified Rhodosporidium toruloides







**Z**умоСнем

NEXT-GENERATION MICROBES FOR INDUSTRIAL CHEMICALS





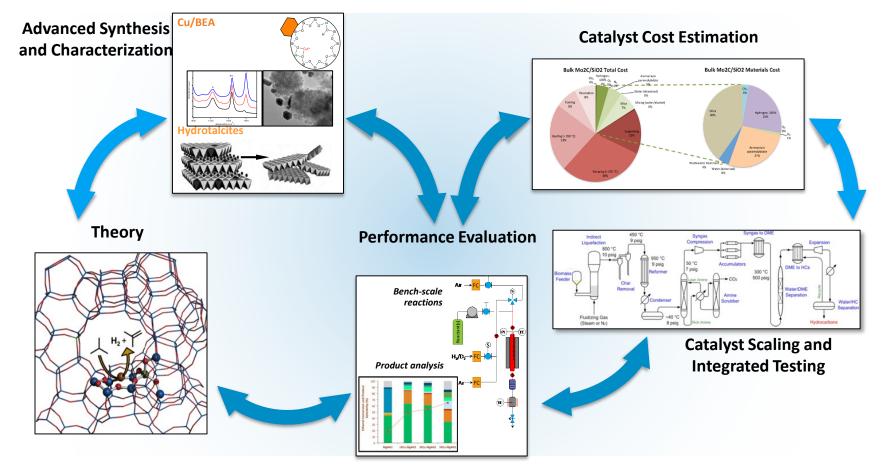




# Establish an integrated and collaborative portfolio of catalytic technologies and enabling capabilities

**Foundational Science** 

Applied Engineering







 NREL has developed atomic layer deposition (ALD) coatings that improve catalyst stability during the production of biobased chemicals, with potential to favorably impact process economics. Through the ChemCatBio DFA, these ALD coatings were recently tailored to improve catalyst performance in the presence of biogenic impurities.



#### Impact in the words of industry:

"The work being done by the NREL team in the ChemCatBio project is of significant value in being able to understand the potential of ALD coating as a tool for next generation catalysts in biomass processing." -Mike Watson "The collaboration with NREL is an extremely valuable method to get industrial validation to the emerging applications for advanced catalyst thin film coatings." -Karen Buechler, CTO of ALD NanoSolutions

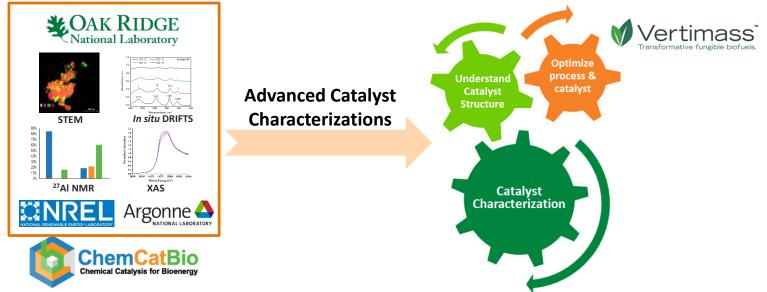
Technology Manager at Johnson Matthey

Work currently under review for publication. A.E. Settle, N.S. Cleveland, X. Huo, A.M. York, E.J. Kautz, A. Devaraj, K.K. Ramasamy, R.M. Richards, K.A. Unocic, G.T. Beckham, M.B. Griffin, K.E. Hurst, E.C.D. Tan, S.T. Christensen, D.R. Vardon. Atomic layer deposition for improved catalyst durability during the production of biobased adipic acid.





The project team at ORNL, NREL and ANL utilized unique characterization techniques to study catalysts used in ethanol upgrading process at Vertimass LLC.



- Deep characterization is helping optimize the catalysts and process, lower cost
  - Identified catalyst changes at various operation conditions
    - Certain operational parameters can effect catalyst performance
    - Characterization provides structure-performance relationship, allowing for process and catalyst optimization

# Impact in the words of industry:

"The ChemCatBio program has provided excellent catalyst characterization insights allowing us to optimize performance and lower conversion costs." -John Hannon, Chief Operating Officer at Vertimass LLC





- The CCPC has developed coupled particle and reactor scale models that have been extensively validated at NREL.
- Recently, these models were leveraged in a collaboration with Forest Concepts to predict required thermochemical conversion times and expected product yields as a function of specific feedstock attributes.



#### Impact in the words of industry:

"The work that you are doing has two direct benefits to our company and the industry. First, the simulations and associated graphics help us understand and explain how the 'dials we turn in production' affect feedstock functional performance. Second, we may want to add new 'label information' to our production reports related to functional performance as well as the physical properties measurements that we currently provide our customers and clients."

-Jim Dooley CTO of Forest Concepts <u>forestconcepts</u><sup>™</sup>



⊙<sub>O</sub>O<sub>O</sub>bioenergy

Methods are reported in: M. Pecha, E. Ramirez, G. Wiggins, D. Carpenter, B. Kappes, S. Daw<sup>2</sup>, and P. Ciesielski, "Integrated Particleand Reactor-Scale Simulation of Pine Pyrolysis in a Fluidized Bed," *Energy&Fuels, 2018* 



# CatCost: Better Cost Information for Catalyst R&D





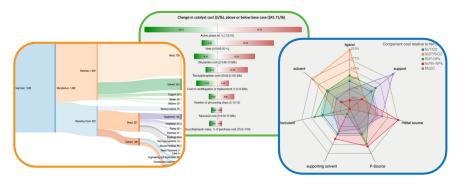


#### Problem: High commercialization risk

- Catalyst cost is a major contributor to commercialization risk for catalytic processes
- Up to 10% of capital cost and  $\pm$  10% uncertainty in MFSP for biomass conversion
- No publicly available tools to evaluate cost

#### Solution: "CatCost" Catalyst Cost Estimation Tool

- Enables early-stage comprehensive cost analysis
- No process design / TEA experience needed
- Improves cost-responsiveness of catalyst R&D



Developed at NREL and PNNL with guidance of industry experts

# Free and public release:

01 October 2018 (debuted at

AIChE meeting's dedicated session)

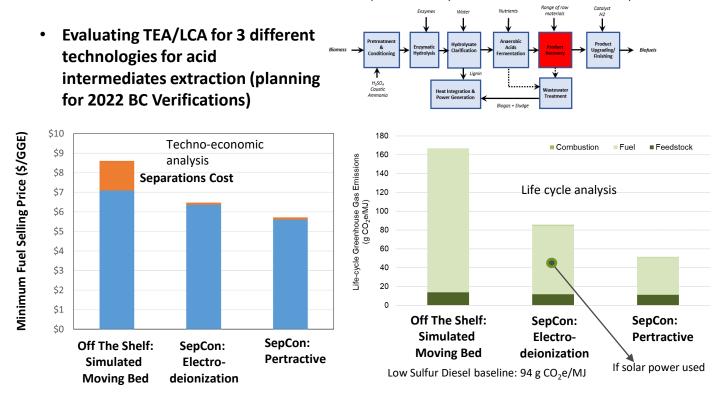
catcost.chemcatbio.org

#### Excel- and web-based versions available

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	Stoichiometric Ratio AP/metal			?					
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	Active Phase Mass at Prep Scale	0.0200	kg						
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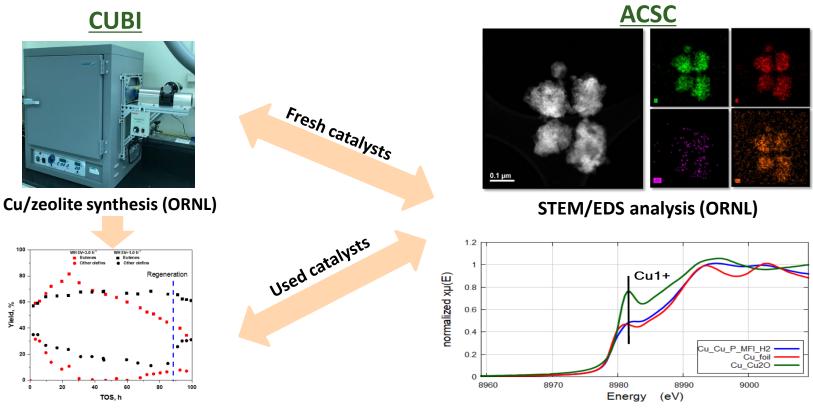
#### Strategies being developed under separations consortium lower separations costs and biofuel lifecycle GHG emissions for this pathway

NOTE: Results reflect scenario in which lignin combusted, resulting energy consumed in process.



CUBI and ACSC collaboration: key to identifying catalyst structure and informing better operation for 2,3-BDO Upgrading





2,3-BDO conversion to butenes (ORNL)

X-ray absorption near edge structure (ANL)

- ACSC helped understand catalyst structure and inform better catalyst operations
  - STEM/EDS: uniform Cu distribution, no large agglomeration
  - XAS: metallic Cu (majority), particle size ≈ 0.7-1.2 nm
  - Frequent catalyst regeneration (<90 h each cycle): avoid hard coke formation
- Major impact: better catalyst design to increase higher olefins yield and lower MFSP



#### **Biological Deconstruction**

• At NREL, moved from batch to continuous countercurrent deacetylation



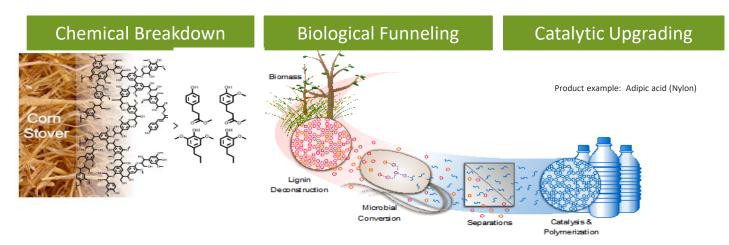
- NREL's Low Temperature Advanced Deconstruction studied how DMR (deacetylation and mechanical refining: the planned pathway for 2022 verification) impacts lignin
  - Used NMR, GPC, and TOF MS to demonstrate that DMR black liquor stream contains large amounts of lignin monomers/dimers along with aryl-ether bonds ( $\beta$ -O-4 linkages intact)
- NREL's Enzyme Engineering and Optimization (EEO) developed an artificial multifunctional cellulase with improved performance over native enzyme mixture
  - NREL has been shifting from DDA to DMR for 2022 cost targets, because DMR's lignin is more readily converted to products
    - But DMR cellulose is more recalcitrant than DDA cellulose
      - So EEO has been developing new cellulases to handle DMR cellulose



### **Biological Upgrading**

- NREL Bench Scale Integration's (BSI) end of year SMART milestone goal was to produce 75 g/L of 2,3-butanediol (BDO) from recombinant Zymomonas mobilis strain fed biomass sugars. BSI exceeded this goal, producing an average of 83 g/L BDO from triplicate fermentations, using a combination of concentrated hydrolysate liquor from deacetylated disc refined (DDR) corn stover, using a fed-batch fermentation strategy, and lowering the aeration rate during xylose metabolism to maximize BDO production.
  - Knockout of pyruvate decarboxylase gene enabled eliminating ethanol pathway
  - Data was produced too late in year to be included in FY18 SOT, but moves BETO closer to the 102 g/L that is targeted in the design case (as a route to \$2.5/gge) and nearly a 2X increase from the end of FY17.
  - Yield was ~86% of theoretical (ultimate project goal is 125 g/L @ 85% yield).
  - In Q1, NREL will deliver 100 L of this fermentation broth to the CUBI teams
- NREL's Biological Upgrading of Sugars (BUS) worked with BioESep to develop in situ product recovery of butyric acid produced from Clostridium, as the Clostridium produces the acid but before cytotoxicity kicks in at high titer
  - Fermentation broth continuously pumped to membrane contactors; cells recycled
  - Extractant in contactors extracts acids; acids then distilled and extractant recycled
  - 300-hr continuous run  $\rightarrow$  +22% productivity and +7% yield of butyric acid





Residual Biorefinery Lignin



Motivation: Lignin constitutes 15-40% of biomass carbon but it is currently considered a waste-stream in biorefineries, generally burned for heat and power.

Techno-economic modeling at NREL has indicated that lignin valorization to high-value products may reduce lignocellulosic biofuel cost by ~\$1-2/gge.

FY18 FOA Selections on conversion of lignin to higher-value products:

- Two awards, \$3.4 million
- Carbon fiber and spray insulation, thermoset polymers used for fiberglass and automotive applications

DOE/USDA Biomass Research and Development Initiative (BRDI) awarded and started to develop a solvent liquefaction process for feedstock deconstruction and lignin upgrading





#### Chemical Breakdown

New flow system gives >35% yield of upgradable monomers with >90% enzymatic hydrolysis yields for monomers

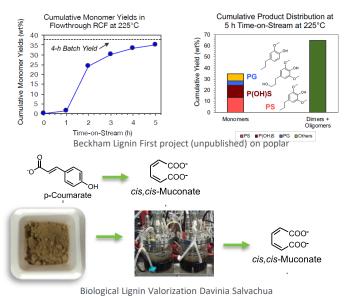
#### **Biological Funneling**

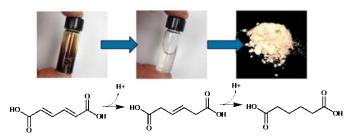
Model feed: 50 g/L titer, 100% yield, 0.5g/L/hr productivity

Real Lignin Baseline First Test:4g/L, 15% yield by mass (137% yieldfrom 2 major monomers in stream)

#### Catalytic Upgrading

>99% yield of adipic acid from biologically produced muconic acid in flow system





Derek Vardon



Energy Efficiency & Renewable Energy

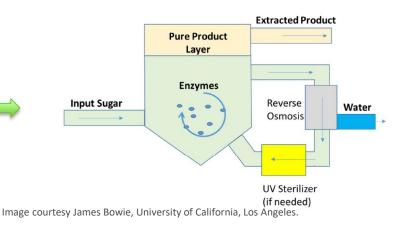
# New/Expanded Areas Since Last Peer Review





#### **Cell-Free Synthetic Biology and Biocatalysis**

- Cell-Free Synthetic Biology as an Enabling Tool for the Bioeconomy
  - Utilizing cell-free synthetic biology as a prototyping tool to rapidly discover the most carbon-efficient and energy-efficient routes from biomass to chemicals
- Cell-Free Synthetic Biology as a New Conversion Platform for the Bioeconomy
  - Free Enzyme Biocatalysis
    - Mix of only the needed enzymes in a reactor could allow better titers, rates, and yields, plus easier product separation
  - Scaffold/Stabilized Biocatalysis
    - Potential novel bioreactor designs such as the "printed tube reactor" (right) for improved mass transfer and heat transfer, compared to traditional designs such as the Continuous Stirred-Tank Reactor



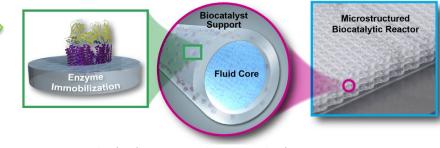


Image courtesy Sarah Baker, Lawrence Livermore National Laboratory.



Energy Efficiency & Renewable Energy

Leveraging DOE's National Laboratories expertise in polymer deconstruction in biomass and applying it to distributed sources of waste carbon to make molecular building blocks for fuels, products, and energy





- BETO-supported National Academies of Sciences study on "Developing a research agenda for utilization of gaseous carbon waste streams"
- CO<sub>2</sub> Valorization via Rewiring Carbon Metabolic Network in bacterial cells
  - NREL tailored bacteria as a model for direct biochemical CO<sub>2</sub> utilization, reaching 150 mg/L titer of 3-hydroxybutyrate (3-HB, a polyester precursor) and developing CRISPR-Cas9 gene editing tools
- Three FY18 FOAs awarded in Topic Area 5: Rewiring Carbon Utilization



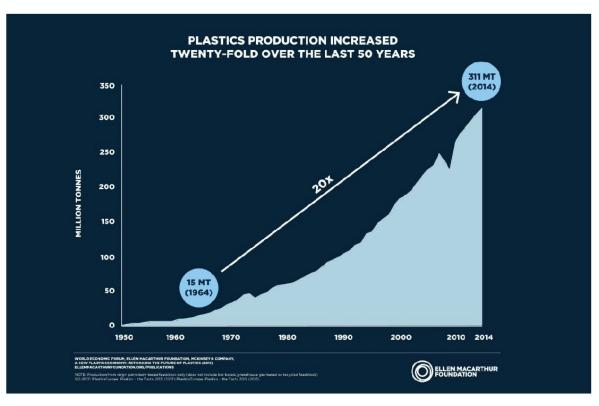
- Formate Lab Call new AOPs in early stage R&D for biological platforms capable of upgrading formate, which can be efficiently generated from CO<sub>2</sub>
  - NREL Improving formate upgrading via bacterial conversion
  - NREL Enhancing CO<sub>2</sub> conversion to value-added products via formate
  - NREL/LBNL Synthetic cycle for electrosynthesis of products and fuels from formate



Plastics are ubiquitous in modern society



#### ~300 MM tonnes per year produced worldwide



Ellen MacArthur Foundation, 2016





#### Plastics are also creating an environmental catastrophe



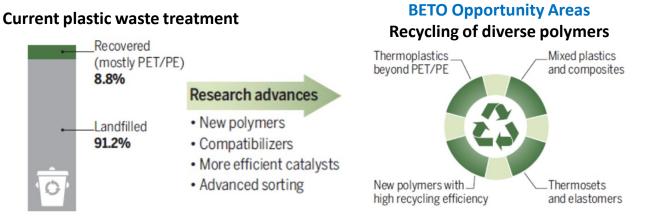
Ellen MacArthur Foundation, 2016





#### Moving beyond PET/PE recycling

Most plastic waste is not currently recycled – New methodologies hold promise for recycling a wider range of plastics, including mixtures.



Garcia, J.M., Robertson, M.L. The Future of Plastics Recycling. Science 358 (6365), 870-872.

**Today's Waste = Tomorrow's Untapped Resources** 



U.S. DEPARTMENT OF

Energy Efficiency & Renewable Energy

Name	Affiliation	Previous Peer Review Experience
Charles Abbas (Lead Reviewer)	iBiocat	New this year
Steve Van Dien	Persephone Biome, Inc.	Reviewer
Ben Gordon	MIT-Broad Foundry	New this year
Chris Rao	University of Illinois at Urbana-Champaign	New this year
Farzaneh Rezaei	Pivot Bio	New this year



Charles





Ben





Farzaneh

## Introductions – Agile BioFoundry Reviewers

U.S. DEPARTMENT OF

Energy Efficiency & Renewable Energy

Name	Affiliation	Previous Peer Review Experience	
Ben Gordon (Lead Reviewer)	MIT-Broad Foundry	New this year	
Matt Tobin	Matthew B. Tobin Consulting	New this year	
Farzaneh Rezaei	Pivot Bio	New this year	
Chris Rao	University of Illinois at Urbana-Champaign	New this year	
Steve Van Dien	Persephone Biome, Inc.	Reviewer	



Ben







Farzaneh



Chris

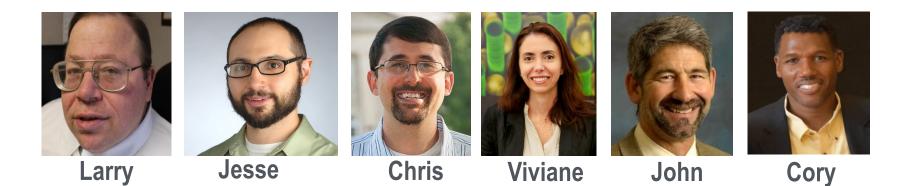


Steve

# Introductions – Catalysis Reviewers



Name	Affiliation	Previous Peer Review Experience
Lorenz (Larry) Bauer	Consultant	TC Reviewer 2017
Jesse Bond	Syracuse University	New, w/MR experience
Chris Bradley Viviane Schwartz	DOE, Office of Science	New, w/MR experience
Cory Phillips	Phillips 66	New
John Regalbuto	University of South Carolina	New, w/MR experience



# Introductions – CO2 Reviewers



Energy Efficiency & Renewable Energy

Name	Affiliation
Alissa Park	Columbia University (lead reviewer)
Jason Ren	Princeton University
Matthew Lucas	Carbon180
Igor Bogorad	Amyris
Matthew Kanan	Stanford University



Alissa



lgor



Matthew K



Matthew L



Jason



Name	Affiliation	Previous Peer Review Experience
Phil Marrone	Leidos, Inc.	Reviewer
Tim Olson	California Energy Commission	New to BETO peer review, has reviewed for DOE
Gary Vanzin	Colorado School of Mines	New to peer review, has reviewed for DOE
Luca Zullo	VerdeNero, Inc.	Lead Reviewer



# Introductions – Separations/Performance Advantaged Bioproducts

U.S. DEPARTMENT OF

Energy Efficiency & Renewable Energy

Name	Affiliation	Previous Peer Review Experience
Joe Bozell (Lead Reviewer)	University of Tennessee	Reviewer
Peter Keeling	Purdue University	New this year
Melissa Klembara	U.S. Department of Energy – Advanced Manufacturing Office	New to reviewing this year, formerly BETO staff
Jeff Scheibel	formerly of P&G	Reviewer
Matt Tobin	Matthew B. Tobin Consulting	New this year
Joe Pet	er Melissa	Jeff Matt

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Name	Affiliation	Previous Peer Review Experience
Emma Master (Lead Reviewer)	University of Toronto	New this year
Joe Bozell	University of Tennessee	Reviewer
Mike Sanford	Formerly of DuPont	New this year
Jeff Scheibel	formerly of P&G	Reviewer
Matt Tobin	Matthew B. Tobin Consulting	New this year





Joe



Mike



Jeff



Matt

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Emma

# Thank you!





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