Bio-Optimized Technologies to keep Thermoplastics out of Landfills and the Environment

DOE Bioenergy Technologies Office (BETO) 2023 Project Peer Review

BOTTLE 1 – Introduction & BOTTLE Overview

April 3, 2023

Technology Session Review Area: Plastics Deconstruction and Redesign

PI: Gregg T. Beckham, BOTTLE CEO, National Renewable Energy Laboratory

Presenters: Gregg Beckham, Meredith Doyle, BOTTLE COO, and Michelle Reed, BOTTLE Project Manager

Science Leadership Team:

Bob Allen, National Renewable Energy Laboratory; Linda Broadbelt, Northwestern University; Alberta Carpenter, National Renewable Energy Laboratory; Eugene Chen, Colorado State University; Taraka Dale, Los Alamos National Laboratory; Jennifer DuBois, Montana State University; Adam Guss, Oak Ridge National Laboratory; Katrina Knauer, National Renewable Energy Laboratory; Andrew Pickford, University of Portsmouth; Yuriy Román-Leshkov, Massachusetts Institute of Technology; Christopher Tassone, SLAC National Accelerator Laboratory; Meltem Urgun-Demirtas, Argonne National Laboratory

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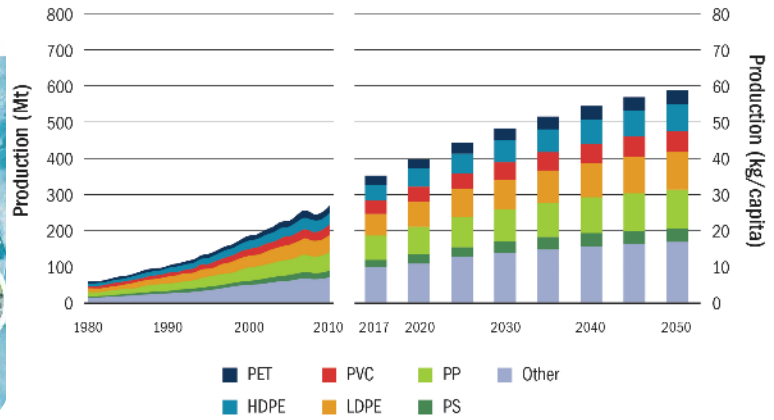
Overview and history of the BOTTLE Consortium

Why should DOE work on plastics circularity?



- ~2% of total energy consumption in the US is used to manufacture plastics, resins, and synthetic rubber
- Plastic production generates ~3.8% of global GHGs
- Plastic production uses ~6% of global oil production, representing a large opportunity for further energy and process efficiency improvements

BOTTLE's history so far…

Oct 2020 — BOTTLE inception

Sept 2021 — BOTTLE kickstarts 2-year project with Amazon

PET enzyme recycling process model
Singh *et al*. *Joule*, 2021

April 2022 — BOTTLE surpasses 100 researchers

Oct 2022 — Demonstrate conversion of PE and PP to propane
Zichittella *et al*. *JACS AU* 2022

Reports oxidation-funneling approach
Sullivan *et al*. *Science* 2022

March 2023 — BOTTLE reports melt-processable PHA materials

U.S. Energy Information Administration. 2021. "2018 MECS Survey Data
Zheng and Suh, *Nature Climate Change* 2019
Ellen MacArthur Foundation. 2017. The New Plastics Economy: Rethinking the Future of Plastics & Catalysing Action

BOTTLE vision, mission, goals, and DEI

Vision

- Deliver scalable technologies that enable cost-effective recycling, upcycling, and energy efficiency for plastics

Mission

- Develop robust processes to upcycle existing waste plastics, and
- Develop new plastics and processes that are recyclable-by-design

Goals

- Work with industry to catalyze new recycling and redesign paradigms
- Leverage DOE investments in process development, catalysis, materials, and analysis-driven R&D

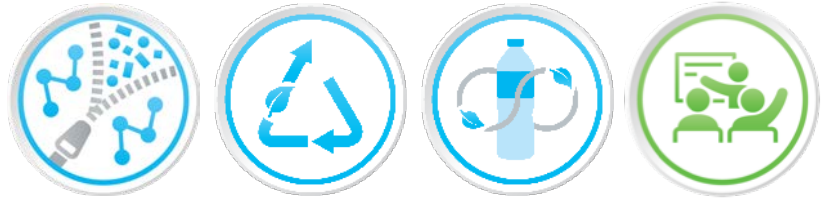
DEI

- A diverse and inclusive consortium that fosters the growth of researchers across their career, engages broadly to educate the public on our work, and ultimately contributes to the local community and the world broadly

Strategic Goals

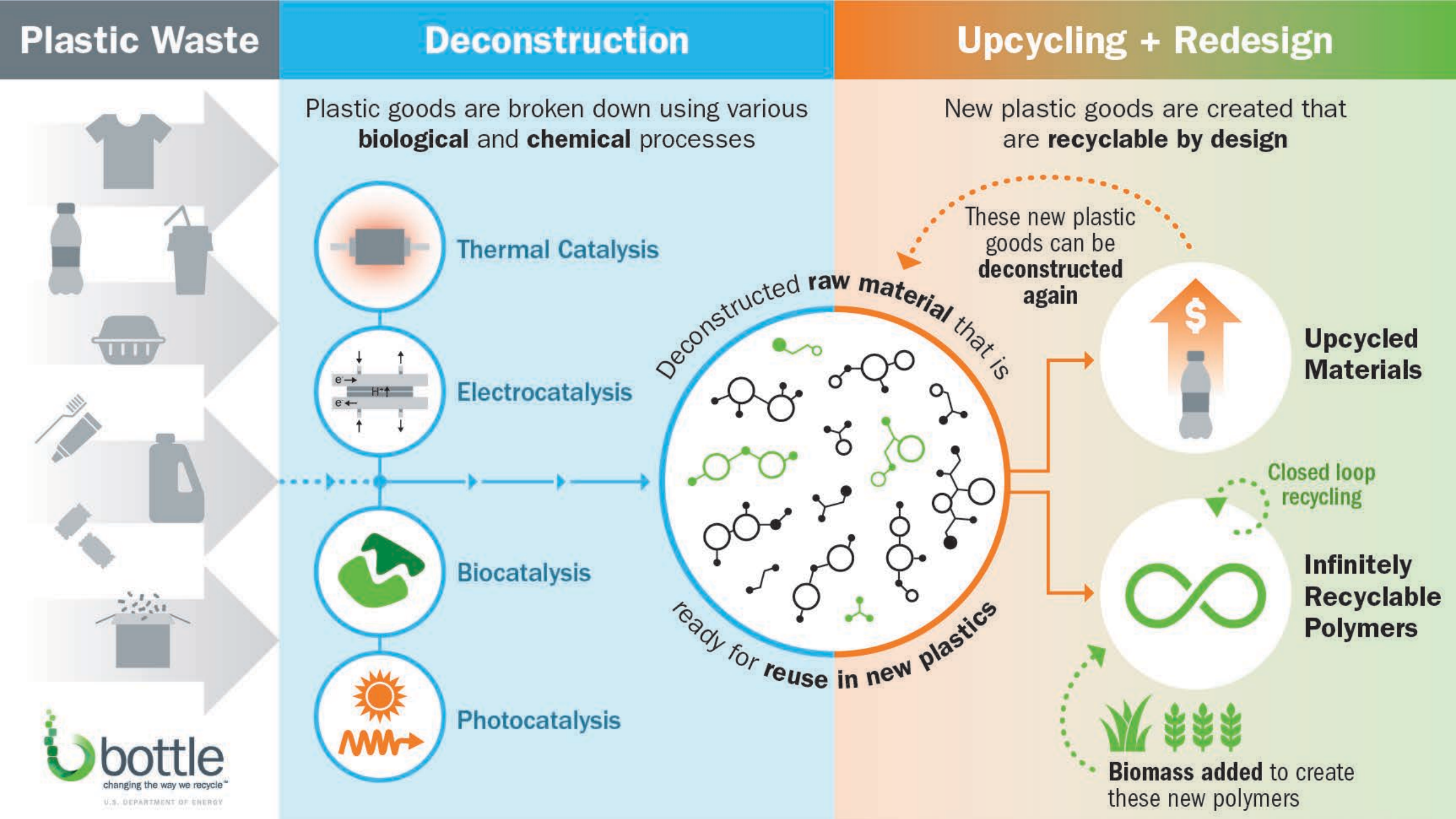
1. **Deconstruction**: Create new chemical, thermal, and biological/hybrid pathways to deconstruct plastics efficiently into useful chemical intermediates.
2. **Upcycling**: Advance the scientific and technological foundations that will underpin new technologies for upcycling chemical intermediates from plastic waste into high-value products.
3. **Recyclable by Design**: Design new and renewable plastics and bioplastics that have the properties of today's plastics, are easily upcycled, and can be manufactured at scale domestically.
4. **Scale and Deploy**: Support an energy- and material-efficient domestic plastics supply chain by helping companies scale and deploy new technologies in domestic and global markets, while improving existing recycling technologies such as collection, sorting, and mechanical recycling.

Aligning BOTTLE tasks:



Deconstruction | Upcycling | Redesign | Industry Engagement

Department of Energy, 2023. Strategy for Plastics Innovation


Plastic Waste
Deconstruction
Upcycling + Redesign
Plastic goods are broken down using various **biological** and **chemical** processes
Thermal Catalysis
Electrocatalysis
Biocatalysis
Photocatalysis
Deconstructed **raw material** that is ready for **reuse in new plastics**
These new plastic goods can be **deconstructed again**
New plastic goods are created that are **recyclable by design**
Upcycled Materials
Closed loop recycling
Infinitely Recyclable Polymers
Biomass added to create these new polymers
bottle
changing the way we recycle
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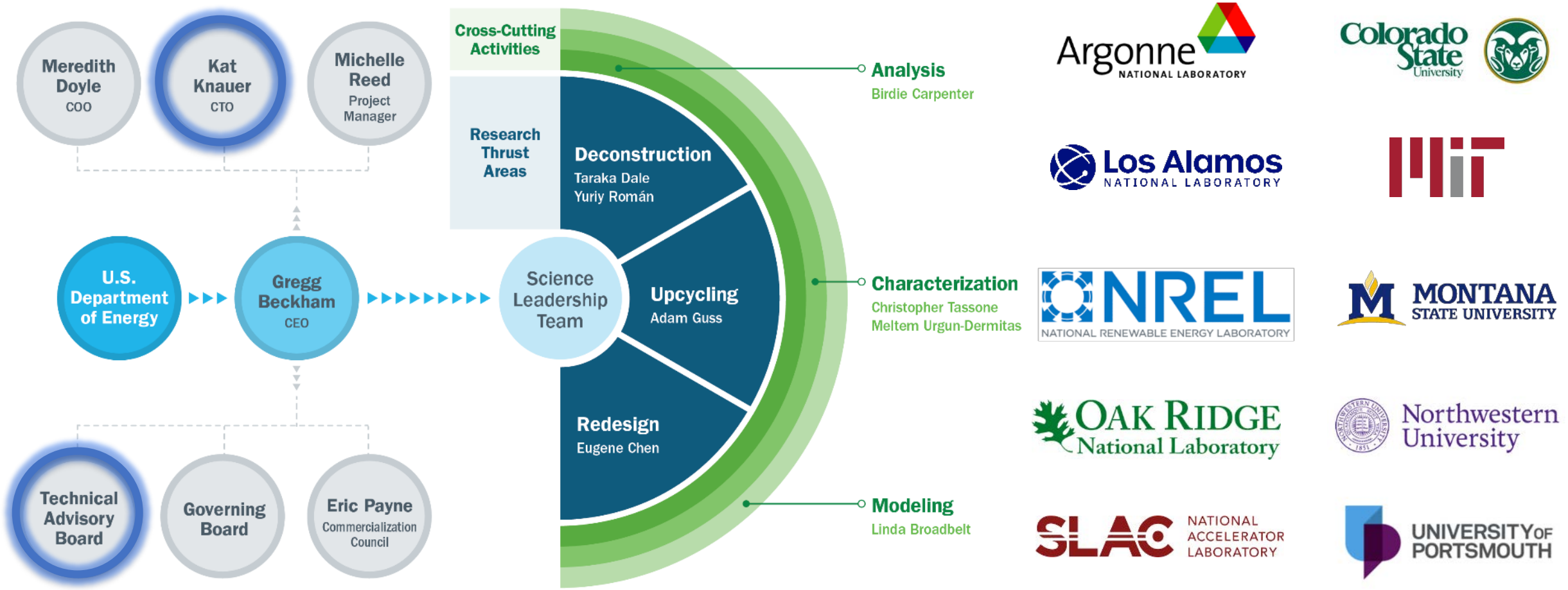
Approach: Team and research task structure



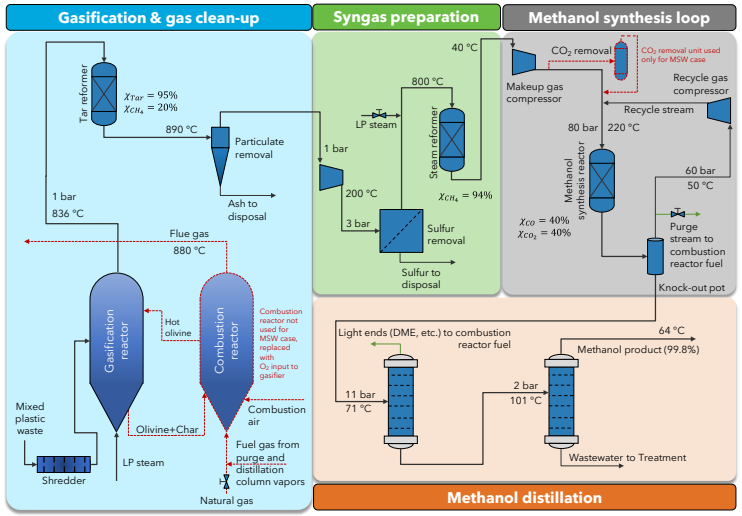
Since FY21, BOTTLE onboarded a Chief Technology Officer (CTO) and Technical Advisory Board (TAB)

Analysis-guided R&D is the foundation of BOTTLE's approach

Example: Gasification of plastic waste to MeOH

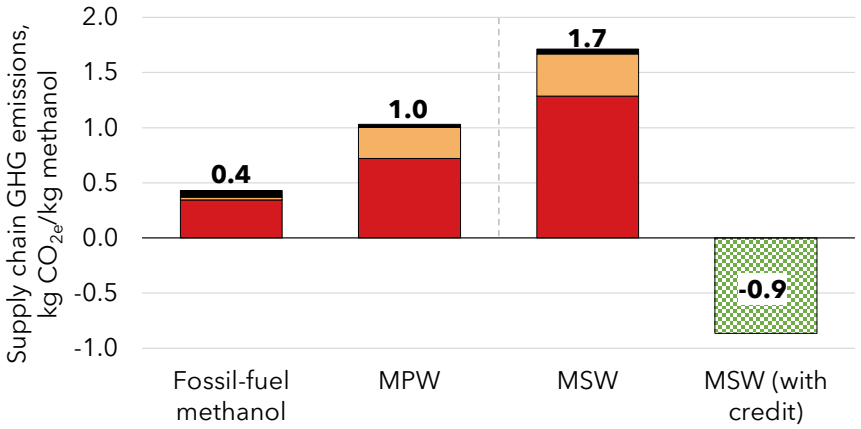
Higher Resolution

Wider Scope



Process modeling & TEA

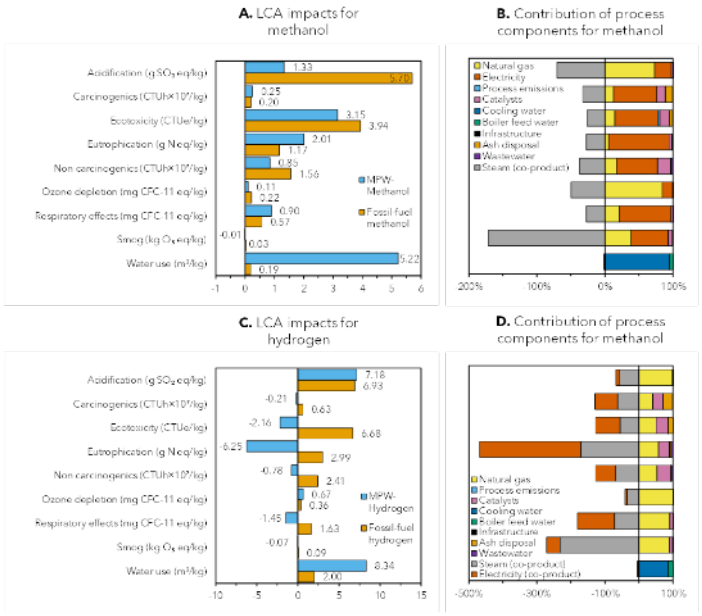
Materials Flows through Industry



Supply chain energy and GHGs

SimaPro

ecoinvent



Comprehensive LCA

Afzal *et al. in revision*

Metrics for BOTTLE projects – Aligning with DOE's SPI

Energy:

- ≥50% energy savings relative to virgin material production
- Closed-loop recycling estimated to save 40-90% energy

Carbon:

- ≥75% carbon utilization from waste plastics
- Estimated based on recycling of commodity thermoplastics

Economics:

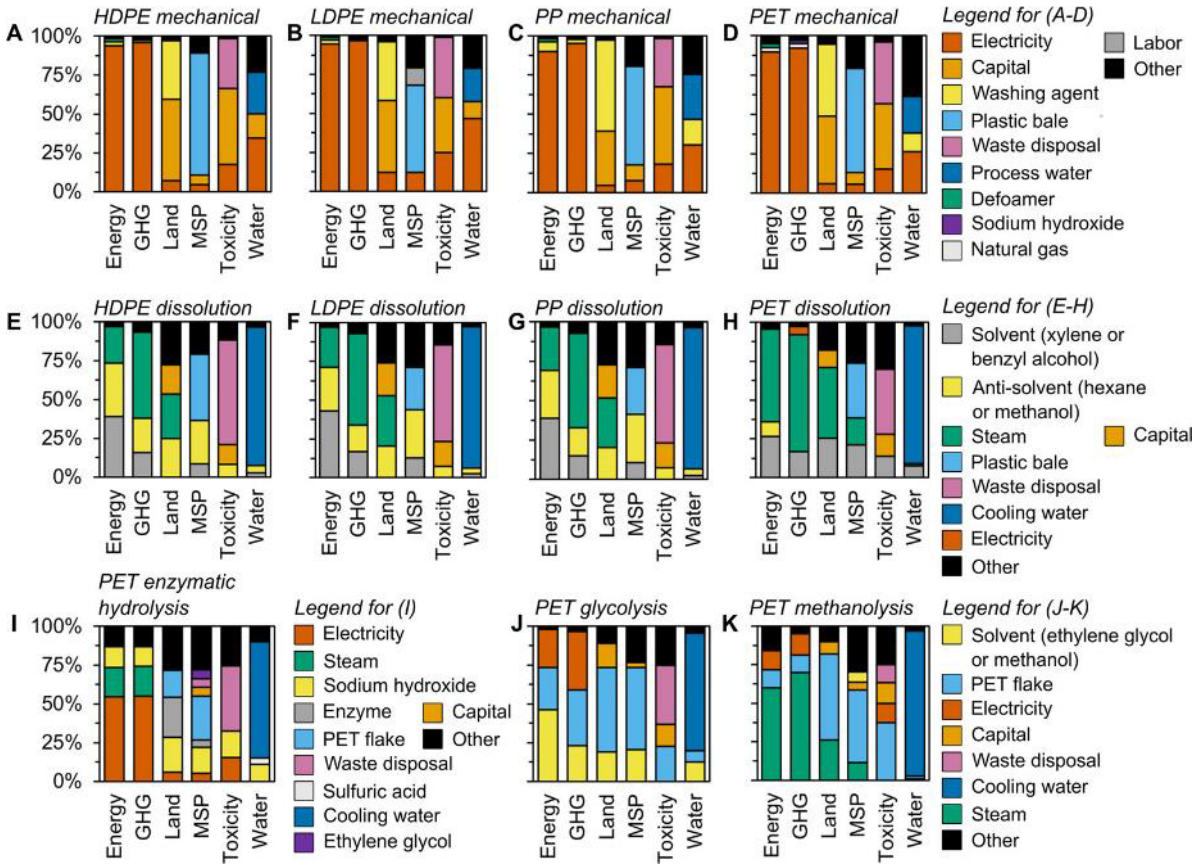
- ≥ 2x economic incentive over reclaimed materials

GHG emissions reductions:

- ≥ 50% GHG emissions reduction compared to virgin manufacturing

Directly aligns to DOE's Strategy for Plastics Innovation (SPI) objectives and metrics

TEA/LCA baseline of current recycling technologies[2]



Uekert *et al. ACS Sustainable Chem. Eng.* 2023; DOE Strategy for Plastics Innovation

Key challenges in BOTTLE's Approach

Challenge 1 – Conducting TEA/LCA across entire BOTTLE portfolio

- Limited data available for early-stage research projects
- Develop best-case scenario initial models

Challenge 2 – Heterogeneity in plastic waste streams

- Consistency challenges in variable feedstocks
- Limited by what is currently collected and sorted or can be sourced
- Key interactions with industry partners

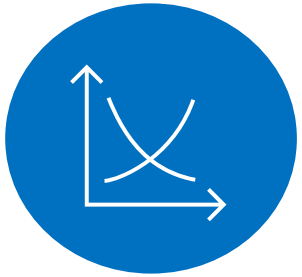
Challenge 3 – Demonstrating scalability to industrial partners at early development stages

- Industrial partners often want a direct line of sight to scale
- Work towards bench-scale integration with real feedstocks as soon as feasible

BOTTLE project risks and mitigation plans

Risk: Limited current capabilities for rapid scaling of promising BOTTLE technologies

Mitigation: Expand interactions within BOTTLE institutions and identify key groups/teams with experience and equipment in scaling and piloting new technologies



Risk: Unable to produce RBD polymers at commodity prices and achieve >50% energy savings relative to today's materials

Mitigation: Conduct analyses of the full polymer life cycle in a linear economy case compared to a circular case to quantify the life cycle energy and economic potential; address monomer manufacturing directly

Risk: The BOTTLE carbon metric might not be achievable in all technology cases

Mitigation: Will evaluate maintaining or off-boarding work when energy and economics metrics are exceeded but carbon metrics cannot be met; will assess relative importance of metrics with comprehensive analysis tools

Collaboration and communication

- Centralized industry engagement and communications efforts

Within BOTTLE:

- Fortnightly BOTTLE R&D meetings include “hot data” and forum for early career researchers to share unpublished work
- Monthly meetings with DOE Technology Managers
- Use Dropbox for data sharing, Slack for communication
- In-person All-Hands meeting with TAB in June 2022
- Shared TAB report with team and updated BOTTLE strategies based on feedback
- Deliver a BOTTLE “portfolio analysis” to BETO/AMMTO Technology Managers to share BOTTLE’s key capabilities

External communication:

- Slack channel with TAB to share papers and updates
- Work with BETO and AMMTO Communications to send out e-blasts on exciting research
- Created BOTTLE Twitter and Instagram accounts

The BOTTLE Consortium & TAB All Hands 2022

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Bioenergy Technologies Office

October 21, 2022

BOTTLE Project Outlines New Two-Step Process for Turning Mixed Plastic Waste into Valuable Bioproducts

BOTTLE Diversity, Equity, and Inclusion (DEI)

Framework complete, developing finalized, detailed plan

BOTTLE's DEI Statement: A diverse and inclusive consortium which fosters the growth of researchers across their career, engages broadly to educate the public on our work, and ultimately contributes to a decarbonized materials economy on both the local community level and the world broadly

Selected DEI Accomplishments to date

Development

- Hiring GEM/SULI interns at multiple BOTTLE labs
- Providing networking and development opportunities for early career researchers
- DEI training for all members planned at All hands
- EJ/SJ speaker series

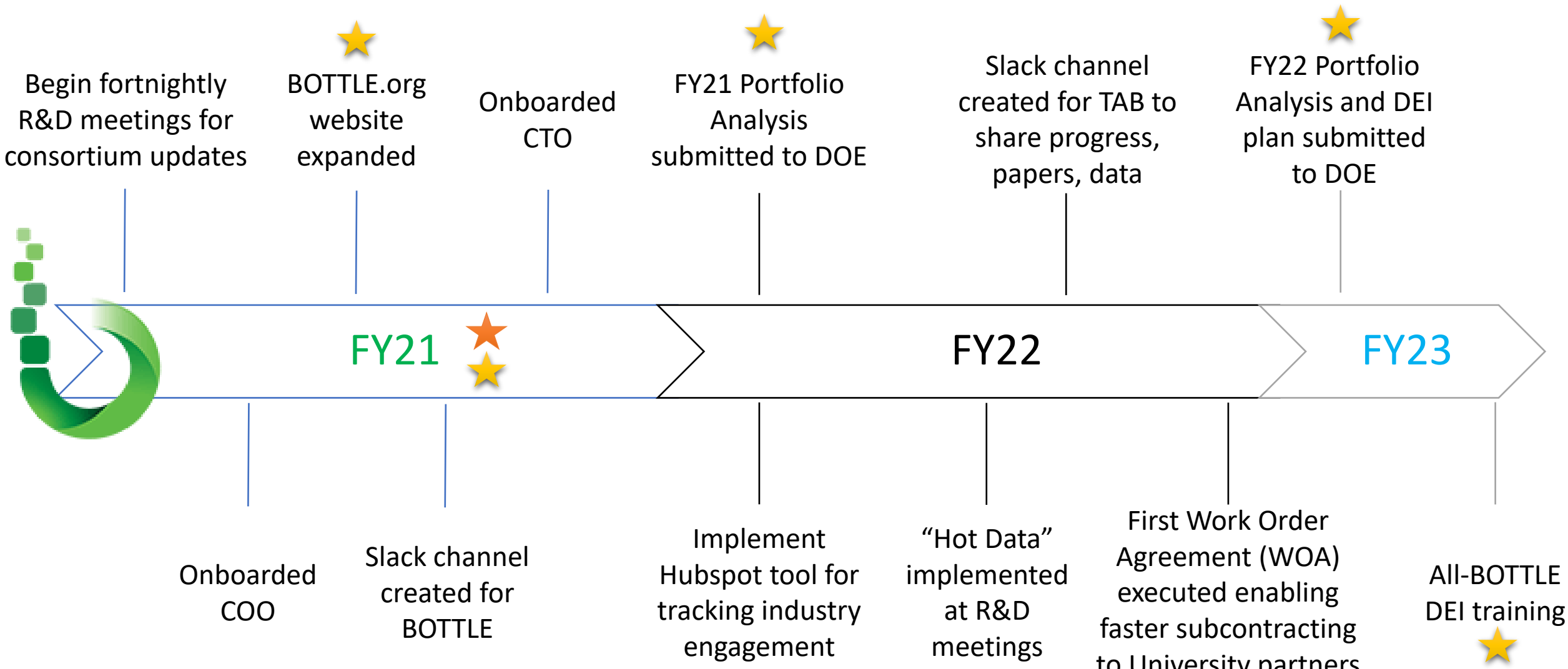
Outreach

- Presentations at MSIs (U Nevada, CCNY)
- Collaboration with an MSI (Hawaiian Pacific)
- Presentations at local high schools
- Participation in URG events (NOBCChE)

Community Change

- Active project to develop a framework to examine Environmental & Social Justice of early TRL technologies into analysis work – will be applied to all BOTTLE projects

Progress: BOTTLE operations

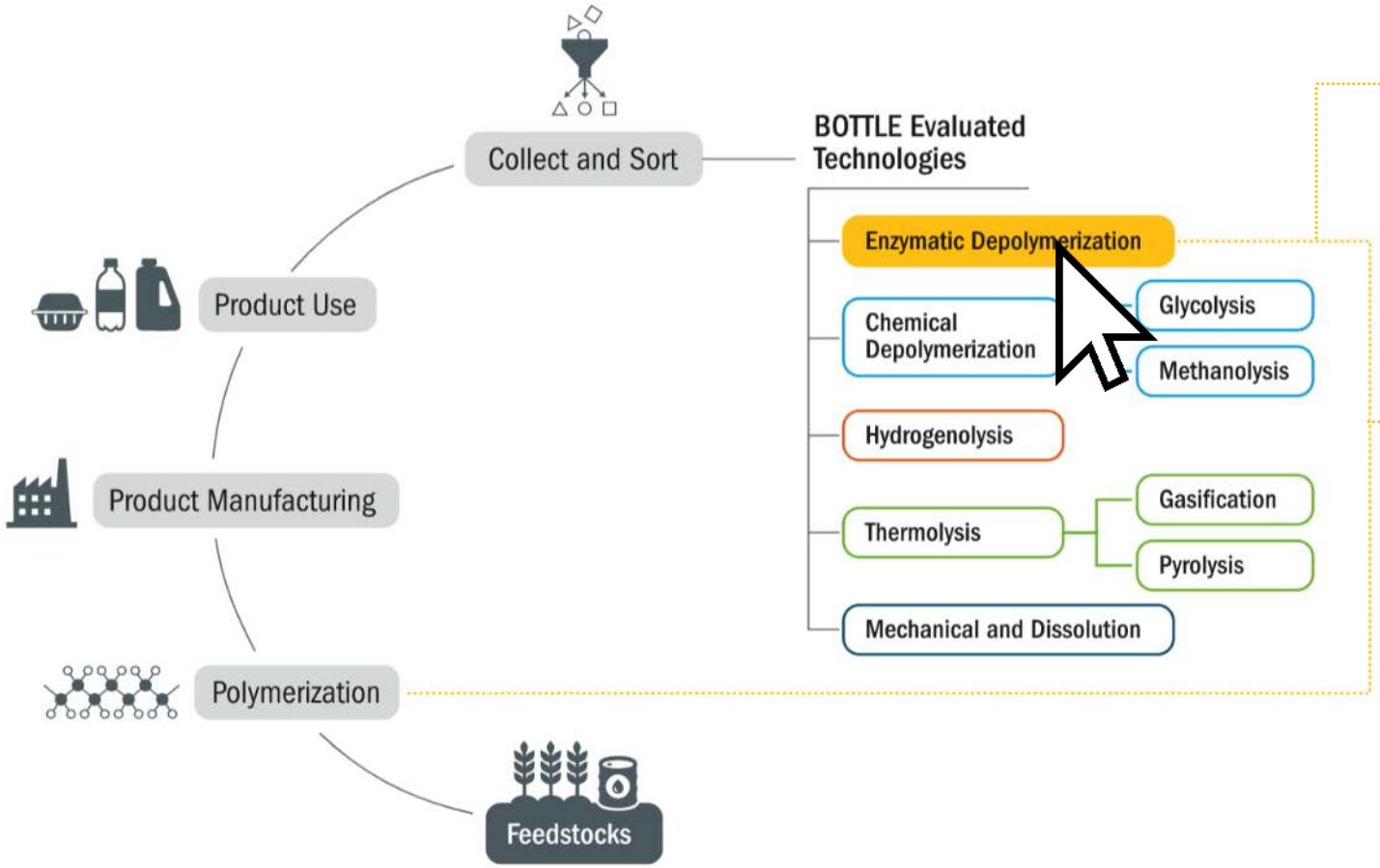


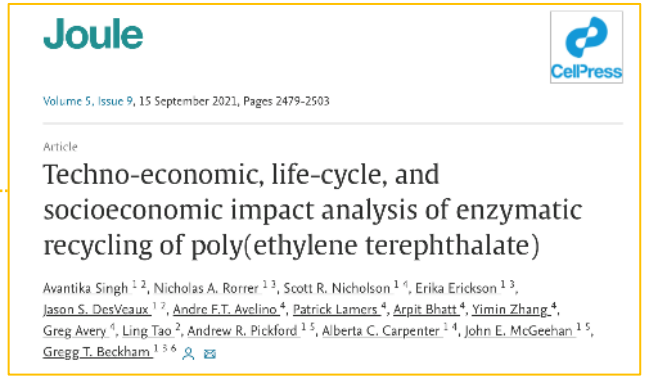
First industry partnership signed

Activity achieved a key BOTTLE milestone

Highlighting analysis-guided research on BOTTLE website

Excerpt from BOTTLE website Analysis page:




Joule

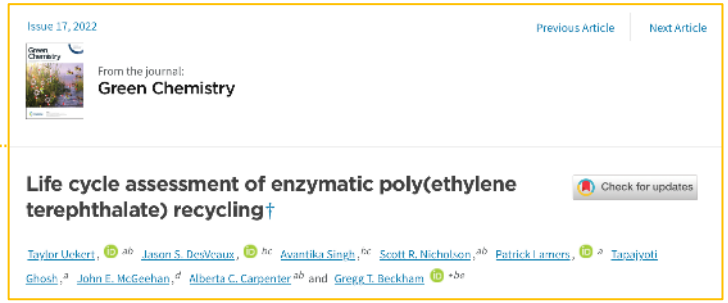
CellPress

Volume 5, Issue 9, 15 September 2021, Pages 2479-2503

Article

Techno-economic, life-cycle, and socioeconomic impact analysis of enzymatic recycling of poly(ethylene terephthalate)

Avantika Singh [1 2], Nicholas A. Rorrer [1 3], Scott R. Nicholson [1 4], Erika Erickson [1 3], Jason S. DesVeaux [1 2], Andre F.T. Avelino [4], Patrick Lamers [4], Arpit Bhatt [4], Yimin Zhang [4], Greg Avery [4], Ling Tao [2], Andrew R. Pickford [1 5], Alberta C. Carpenter [1 4], John E. McGeehan [1 5], Gregg T. Beckham [1 5 6]


Issue 17, 2022

Previous Article | Next Article

From the journal: Green Chemistry

Life cycle assessment of enzymatic poly(ethylene terephthalate) recycling†

Check for updates

Taylor Uekert, [ab] Jason S. DesVeaux, [bc] Avantika Singh, [bc] Scott R. Nicholson, [ab] Patrick Lamers, [a] Tarajyoti Ghosh, [a] John E. McGeehan, [d] Alberta C. Carpenter [ab] and Gregg T. Beckham [*be]

- New interactive figure on BOTTLE website will highlight key Analysis publications
- Viewers can hover over technologies to view pathways in the circular supply chain as well as relevant publications

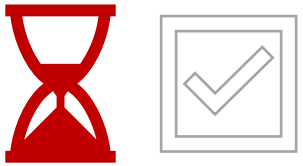
Portfolio analysis within BOTTLE

Using active project management and analysis as a guide, the SLT compiles an annual portfolio review for DOE to evaluate technologies with potential for success and redeploy resources to the greatest opportunities

Summary of decisions to date

Accelerate

- hydrogenolysis for polyolefin deconstruction
- oxidation of mixed plastic waste
- RBD polyethylene
- designer PHAs



Discontinue (or completed)

- photocatalytic deconstruction
- electrocatalytic deconstruction
- biosensor development
- RBD nylons
- hyperbranched polyethylene

Major continuation decisions in FY23

- oxidative deconstruction
- enzymatic deconstruction of PET
- directed evolution for enzymatic deconstruction of PET and nylon
- catalyzed glycolysis of polyesters
- engineering *Geobacillus* for the conversion of PET

BOTTLE's Technical Advisory Board

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Scott Farling

Adrienne Huston-Davenport

Guy Joly

Kara Lavender-Law

Susannah Scott

Brent Shanks

Margaret Sobkowicz-Kline

Mark Spalding

Scott Trenor

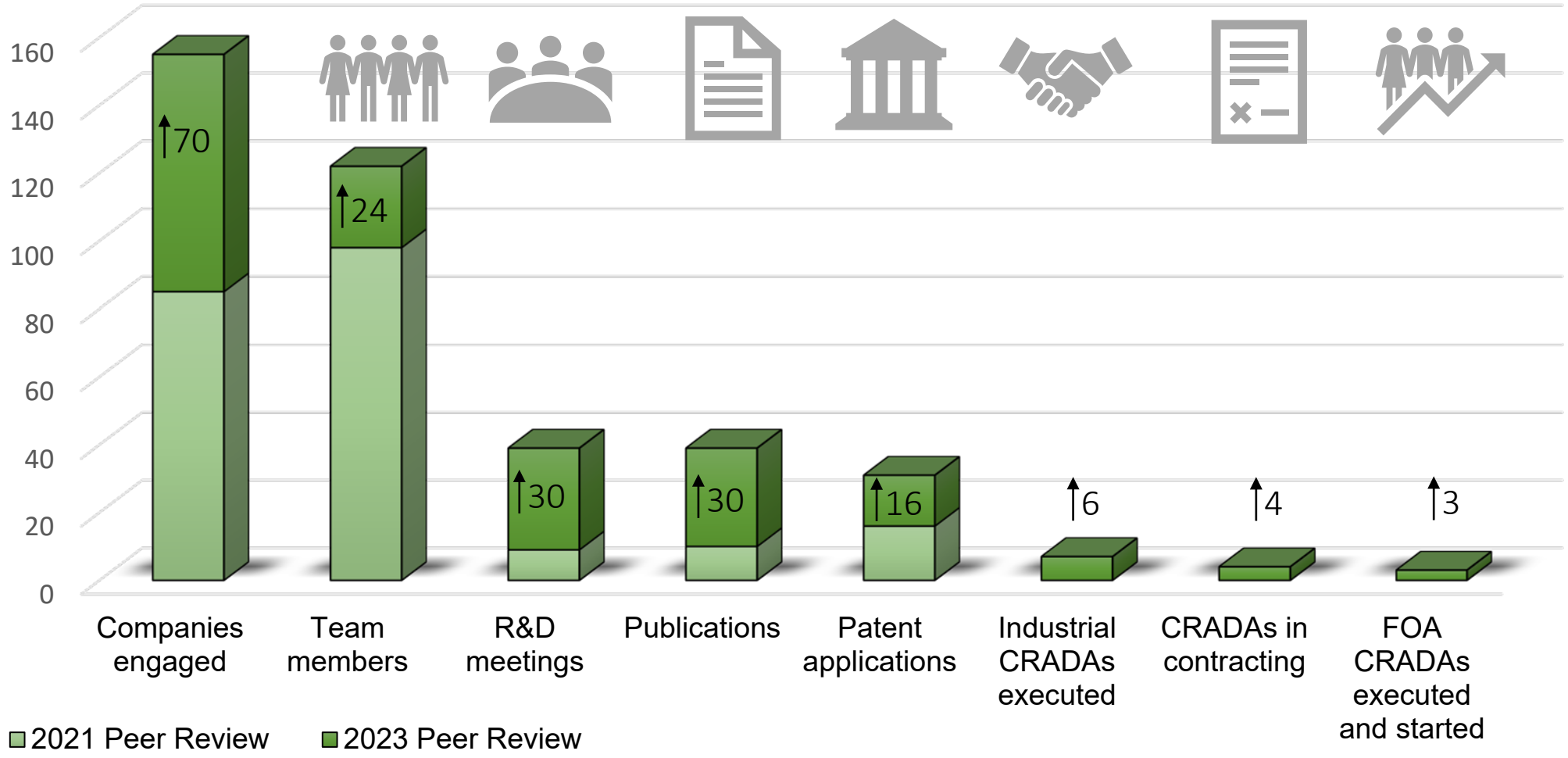
Role of the TAB:

- Feedback on R&D, operations, management
- Convene annually with the All-Hands meeting
- Provide written evaluations to DOE, BOTTLE LT

Excerpt from 2022 Report:

TAB recognized the excellent organization and management, comprehensive and evolving science leadership team, and attention to interdisciplinary teaming to ensure success

Impact: BOTTLE growth



Impact

- Development framework for circularity analysis – attracting engagement from industry, NGOs, and academic partners
- Substrate characterization methods proposed for reproducibility (Ellis *et al., Nature Catal.* 2021)
- Training next-generation leaders in polymer sustainability and conducting active outreach
- Combining chemistry & biology to valorize mixed plastic waste and to produce monomers for recyclable-by-design polymers
- High-impact publications are attracting industrial partners who have identified BOTTLE technologies as promising solutions for plastic deconstruction, upcycling, and redesign

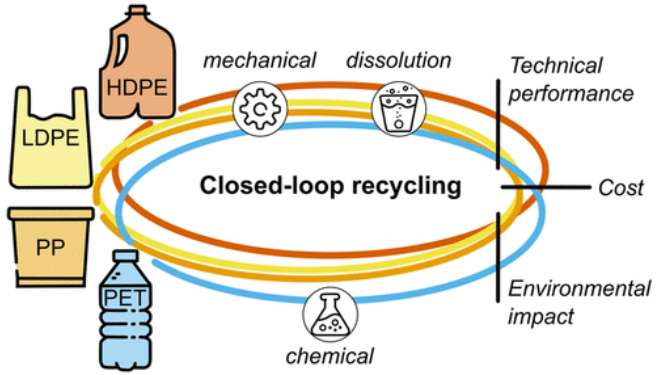


Image from Uekert *et al.*, *ACS Sustainable Chem. Eng.* 2023

Resulted in:
- 4+ industrial contacts
- 32 news outlets

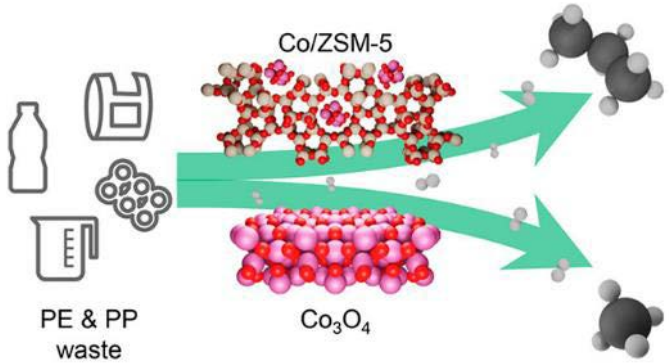


Image from Zichittella *et al.*, *JACS AU* 2023

Resulted in:
- 2+ industrial contacts
- 31 news outlets

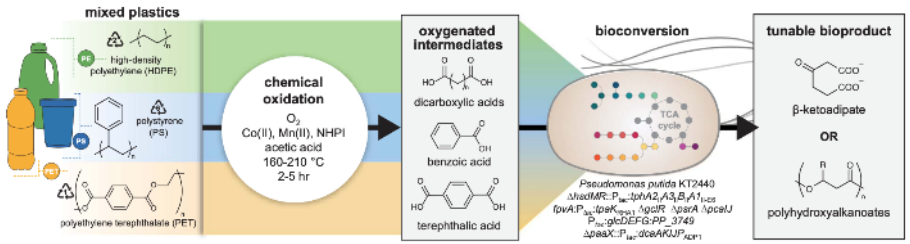


Image from Sullivan, Werner, Ramirez, Ellis, *et al.*, *Science* 2022

Resulted in:
- 10+ industrial contacts
- 80 news outlets

Summary

Overall:

- BOTTLE conducts interdisciplinary, industry-relevant, and process-enabling research to deconstruct and upcycle today's plastics and redesign tomorrow's plastics

Approach:

- BOTTLE is analysis guided and uses a Portfolio Analysis process to on/offboard projects with input from DOE

Progress and Outcomes:

- Onboarded a CTO and Technical Advisory Board
- Drafted a BOTTLE DEI framework

Impact:

- 6 funds-in CRADA industrial partnerships executed, 4 in contracting
- 40 publications, 32 patent applications to date

Thank you!

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bottle

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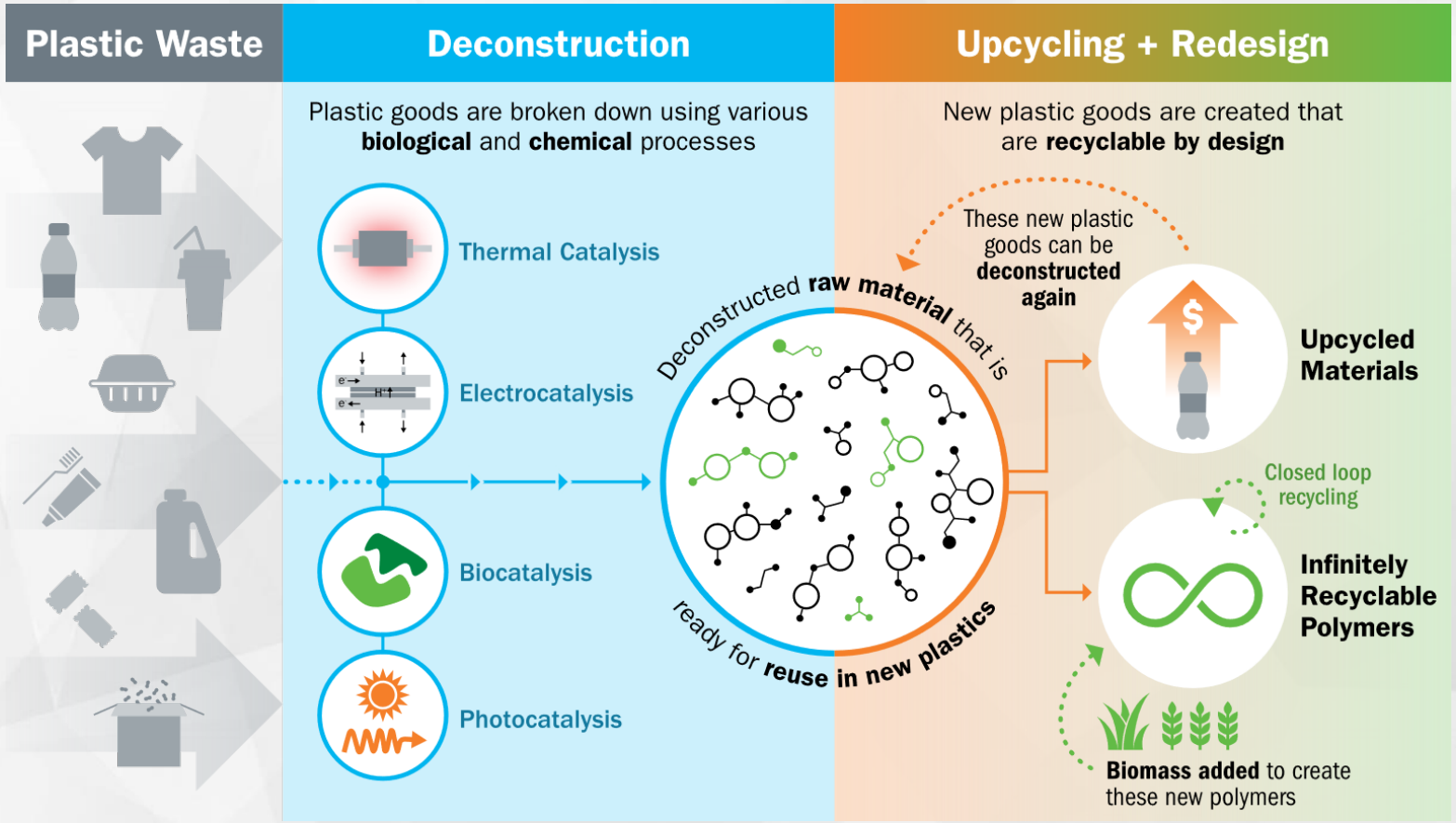
Bio-Optimized Technologies to keep Thermoplastics out of Landfills and the Environment



Q&A

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NREL/PR-2A00-85657

Publications

In preparation

Amy A. Cuthbertson, Clarissa L. Lincoln, Joel Miscall, Lisa Stanley, David T. Moore, Brenna A. Black, Nicholas A. Rorrer, Gregg T. Beckham, Characterization of polymer properties and identification of additives in commercial research plastics, in preparation.

Shaik Afzal, Avantika Singh, Scott R. Nicholson, Taylor Uekert, Eric C.D. Tan, Abhijit Dutta, Robert M. Baldwin, Gregg T. Beckham, Techno-economic analysis of mixed plastic waste gasification for the production of methanol and hydrogen, in preparation for *Energy Env. Sci.*

Rosie Graham, Erika Erickson, Richard K. Brizendine, Davinia Salvachúa, Zhongping Tan, Gregg T. Beckham, John E. McGeehan, and Andrew R. Pickford, Enzymatic deconstruction of poly(ethylene terephthalate) is not improved by the use of carbohydrate-binding modules at industrially-relevant solids loadings, in preparation for *Chem Catalysis*.

Julie E. Rorrer, Amani M. Ebrahim, Ydna Questell-Santiago, Clara Troyano-Valls, Arun S. Asundi, Simon R. Bare, Christopher J. Tassone, Gregg T. Beckham, Yuriy Román-Leshkov, Selective hydrogenolysis of polyethylene and polypropylene waste to liquid hydrocarbons over bifunctional Ru/acid catalysts, in preparation.

Geetanjali Yadav, Avantika Singh, Abhijit Dutta, Scott R. Nicholson, Kylee Harris, Calvin Mukarakate, Joshua A. Schaidle, Cody J. Wrasman, Yuriy Román-Leshkov, Robert M. Baldwin, Gregg T. Beckham, Techno-economic analysis of pyrolysis of mixed plastics waste, in preparation for *Energy Env. Sci.*

Submitted

Houqian Li, Robert D. Allen, Xianglan Bai, Gregg T. Beckham, et al., Expanding plastics recycling technologies: chemical aspects, technology status and challenges, submitted to *ACS SusChemEng.*

Publications

In review

Richard K. Brizendine, Erika Erickson, Stefan J. Haugen, Kelsey J. Ramirez, Joel Miscall, Davinia Salvachúa, Andrew R. Pickford, Margaret J. Sobkowicz-Kline, John E. McGeehan, Gregg T. Beckham, Effect of particle size and substrate crystallinity on enzymatic depolymerization of poly(ethylene terephthalate), in review at ACS SusChemEng.

Kevin P. Sullivan, Allison Z. Werner, Kelsey J. Ramirez, et. al., Tandem chemical oxidation and biological funneling for upcycling of mixed plastic waste, in review at Science.

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Design Principles and Chemocatalytic Methods for Circular Polymers and Biodegradable Plastics, BASF Lecture in Organic Chemistry, November 2022.

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Presentations

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Using redesigned iron catalysts to bring aromatic subunits to a common intermediate, SIMB 2022, August 2022

Techno-economic analysis and life cycle assessment for catalytic fast pyrolysis of mixed plastic waste, BioEnergy TRP Meeting, National Renewable Energy Laboratory, August 2022.

Bio-based, recyclable-by-design polymers, ACS National Meeting, August 2022

Presentations

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High throughput test tools for industrially relevant microbial chassis, SIMB 2022, August 2022.

Circular polymers and biodegradable plastics, Circular Polymers and Biodegradable Plastics International Research Training Group, University of Muenster, July 2022.

Engineering P450s to alleviate a bottleneck to lignin demethylation, Intl. Conference on Porphyrins and Phthalocyanines, July 2022.

Difficult to recycle plastics, Sustainable Packaging Coalition Engage Meeting, July 2022.

Selective chemical recycling of mixed plastics waste, Polymer Physics Gordon Research Conference, July 2022.

Plastics recycling and upcycling in the BOTTLE Consortium, NASEM Committee on Repurposing Plastic Waste, July 2022.

Developing strategies for polymer redesign and recycling using reaction pathway analysis, Gordon Research Conference on Polymer Physics, July 2022.

Multi-Material Flexible Packaging Coalition SPC, February 2022.

Presentations

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Development of chemical recycling approaches for plastic waste, Enzyclic Consortium (via webinar), January 2022

Development of chemical recycling approaches for plastic waste, UIUC, December 2021

Design Principles and Synthetic Methodologies for Circular Polymers with Intrinsic Recyclability and Tunable Properties, Pacifichem Conference, December 2021

New building blocks for performance-advantaged renewable and recyclable polymers, Pacifichem (via webinar), December 2021

Discovery and characterization of PET degrading enzymes, University of Rochester microplastics workgroup seminar series, December 2021.

Design Principles and Synthetic Methodologies for Intrinsically Circular Polymers and Biodegradable Plastics, Columbia University, November 2021

Selective Hydrogenolysis of Polyethylene and Polypropylene to Liquid Alkanes over Tunable Ruthenium-Based Heterogeneous Catalysts, 2021 AIChE National Conference, Boston, MA, November 2021.

Plastics recycling and upcycling, ACS Converge (via webinar), October 2021

Presentations

Genetic tools and microbial engineering for biological production of sustainable fuels and chemicals, Presented to Weekly Seminar for DOE CCI/SULI Students. October 2021

Heterogeneous Catalytic Deconstruction and Upcycling of Waste Polyolefins, Biodesign Institute at Arizona State University, SM3 Seminar Series, October 2021.

Domestication of diverse non-model microbes for plastics upcycling and sustainable fuel and chemical production, Biological Sciences Departmental Seminar, Michigan Technical University. October 2021.

Catalysis for valorization of lignin and plastics, Great Plains Catalysis Society (via webinar), June 2021

The critical role of economic and environmental analysis to guide research in lignin valorization and plastics upcycling, Keynote Invited Lecture, ACS Green Chemistry and Engineering (via webinar), June 2021

Towards Intrinsically Circular Thermoplastics and Reprocessable Thermosets, Dow Chemical Company, virtual seminar, May 2021

Recent progress in performance-advantaged bioproducts and plastics upcycling, Arizona State University (via webinar), April 2021

Recent adventures in biomass conversion and plastics upcycling, Rutgers University (via webinar), April 2021

Presentations

Recent adventures in biological plastics upcycling, MIX-UP Consortium (via webinar), April 2021

Framing challenges and opportunities for chemical recycling of waste plastics, ACS Presidential Symposium on Chemistry and the Future of Plastics (via webinar), April 2021

Recent updates in plastics upcycling from the BOTTLE Consortium, ExxonMobil Research and Engineering, April 2021

Design Principles and Synthetic Methodologies for Circular Polymers and Biodegradable Plastics, KAUST, Physical Science and Engineering Division, virtual seminar, April 2021

Heme and non heme iron enzymes and renewable carbon, University of San Antonio Texas, April 2021

A flexible kinetic assay efficiently sorts potential biocatalysts for BHET hydrolysis, Symposium on Biomaterials, Fuels, and Chemicals, April 2021

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Design Principles for Circular Plastics with Tunable Properties, CellPress LabLinks: The Circular Plastics Economy: Linking Across Scales, virtual event with 440 registered attendees. March 2021.

Process analysis for enzymatic PET recycling, Global Research and Innovation on Plastics annual meeting (via webinar), March 2021

Presentations

Polyolefin upcycling in the BOTTLE Consortium, Annual SPE meeting (via webinar), February 2021

Biological processes for lignin and plastics conversion, University of California Riverside (via webinar), January 2021