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

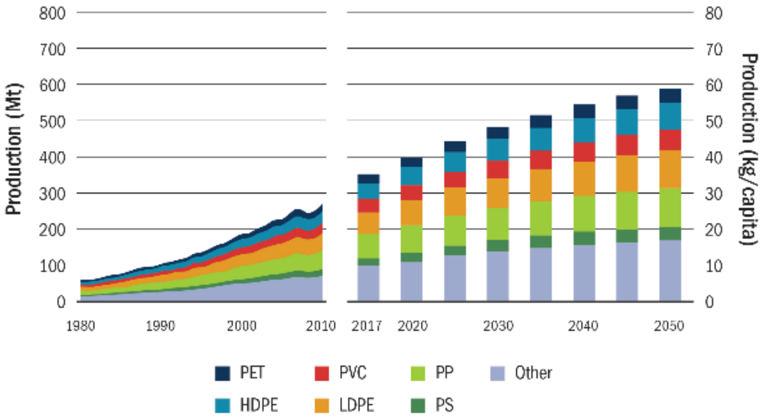
BOTTLE Consortium | AMMTO
May 16th, 2023

Gregg T. Beckham, BOTTLE CEO, National Renewable Energy Laboratory
WBS 2.1.0.52 | 10/1/2021 – 9/30/2023

AMMTO & IEDO Joint Peer Review
May 16th-18th, 2023
Washington, D.C.

Project overview

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

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

Cross-cutting BOTTLE tasks:

Analysis Modeling Characterization

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

Department of Energy, 2023. Strategy for Plastics Innovation

Project outline

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

These innovations will position the US as a global leader in advanced plastics recycling technologies and in the manufacturing of new plastics that are recyclable-by design

Project lead: National Renewable Energy Laboratory

Project partners: Argonne National Laboratory, Los Alamos National Laboratory, Oak Ridge National Laboratory, SLAC National Accelerator Laboratory, Colorado State University, Massachusetts Institute of Technology, Montana State University, Northwestern University, University of Portsmouth

Timeline: 10/1/2021 – 9/30/2023, 88% progress

Budget:

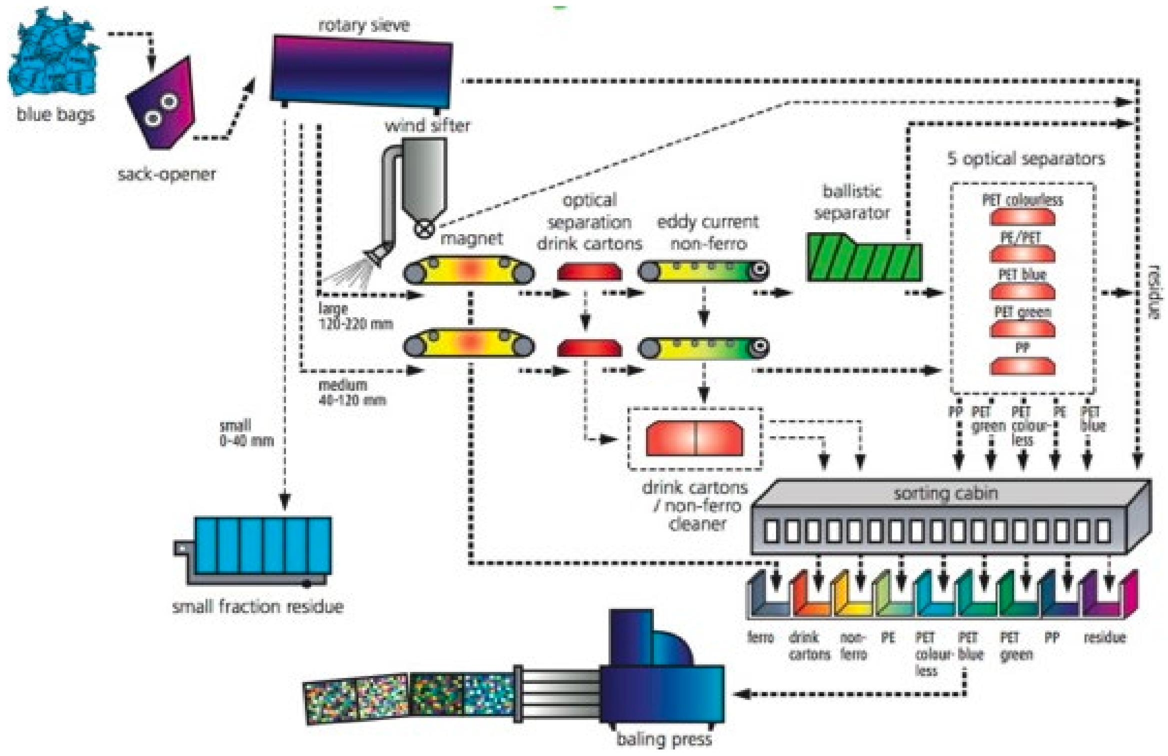
	FY21 Costs	FY22 Costs	FY23 Costs	Total Planned Funding
DOE-funded (AMMTO & BETO)	$10,000,000	$10,000,000	$10,000,000	$30,000,000

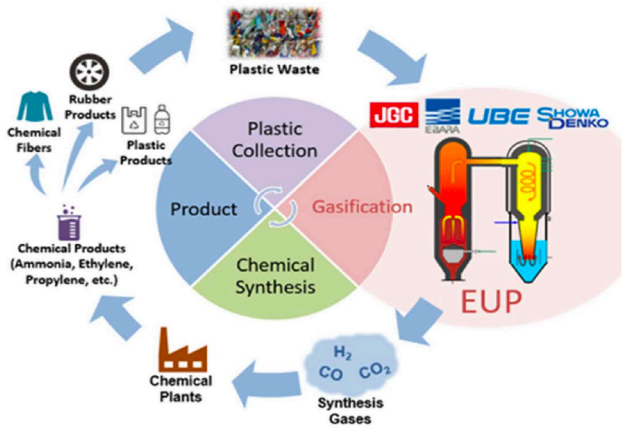
End project goal: Develop selective, scalable processes to deconstruct and upcycle today's plastics and thermosets, redesign tomorrow's plastics to be recyclable-by-design (RBD) and derived from bio-based feedstocks, and work with industry to catalyze new upcycling paradigms and novel feedstocks

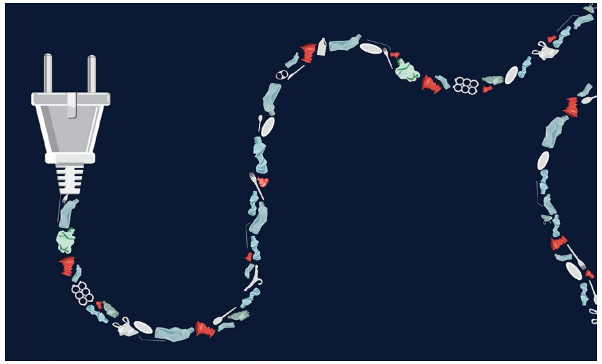
Background

Current plastics waste management and recycling approaches are insufficient:

- Recycled plastics often lower quality and value
- Mech. recycling not applicable to all polymers
- Little economic incentive for plastics reclamation



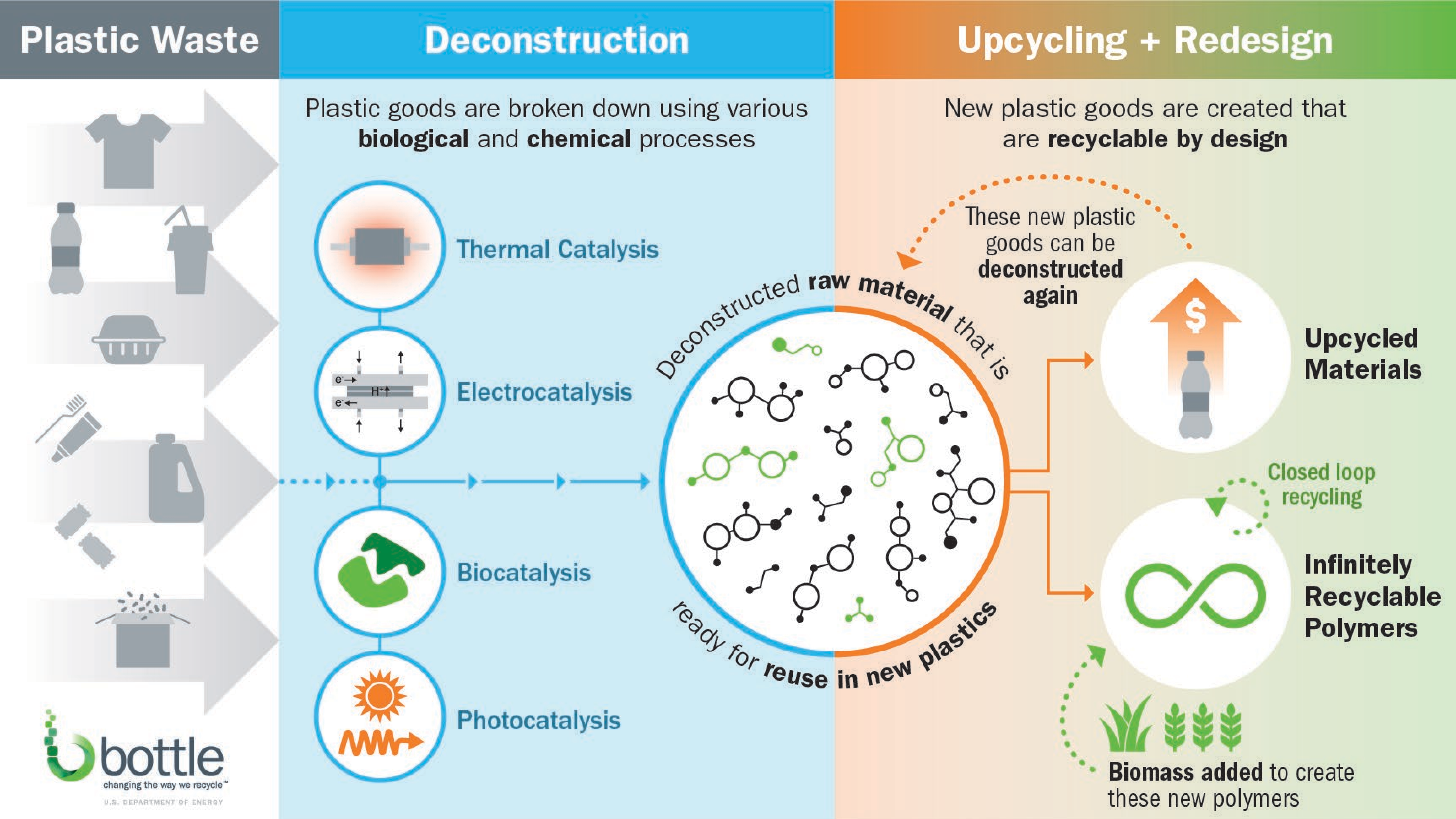




Methods “beyond” mechanical recycling for waste plastics: energy recovery, pyrolysis, and gasification

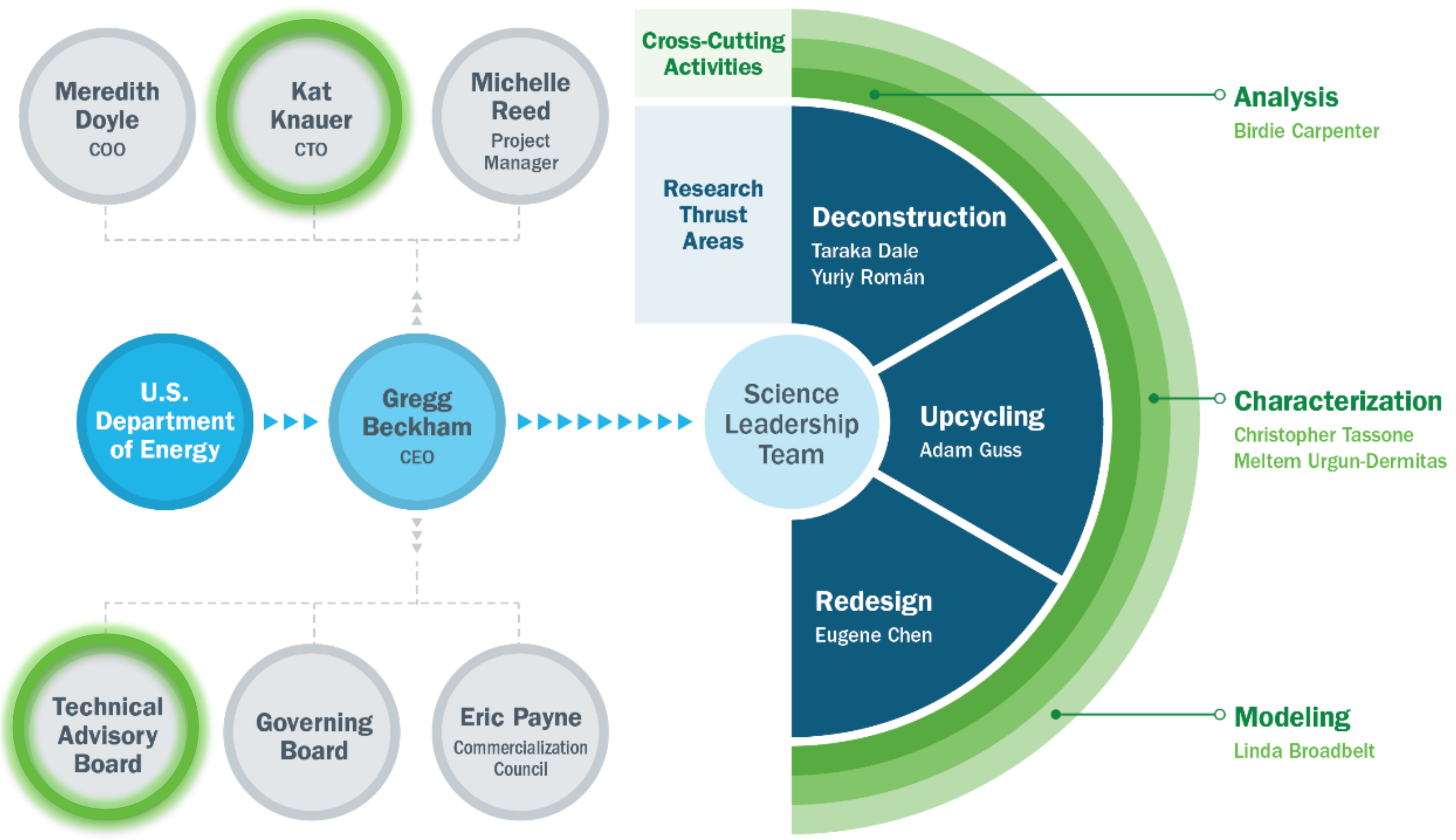
Image from Van Geem *et al. Waste Management* 2017

Images from ChemWeek, Plastics News Europe, C&E News



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

Approach: Team and research task structure

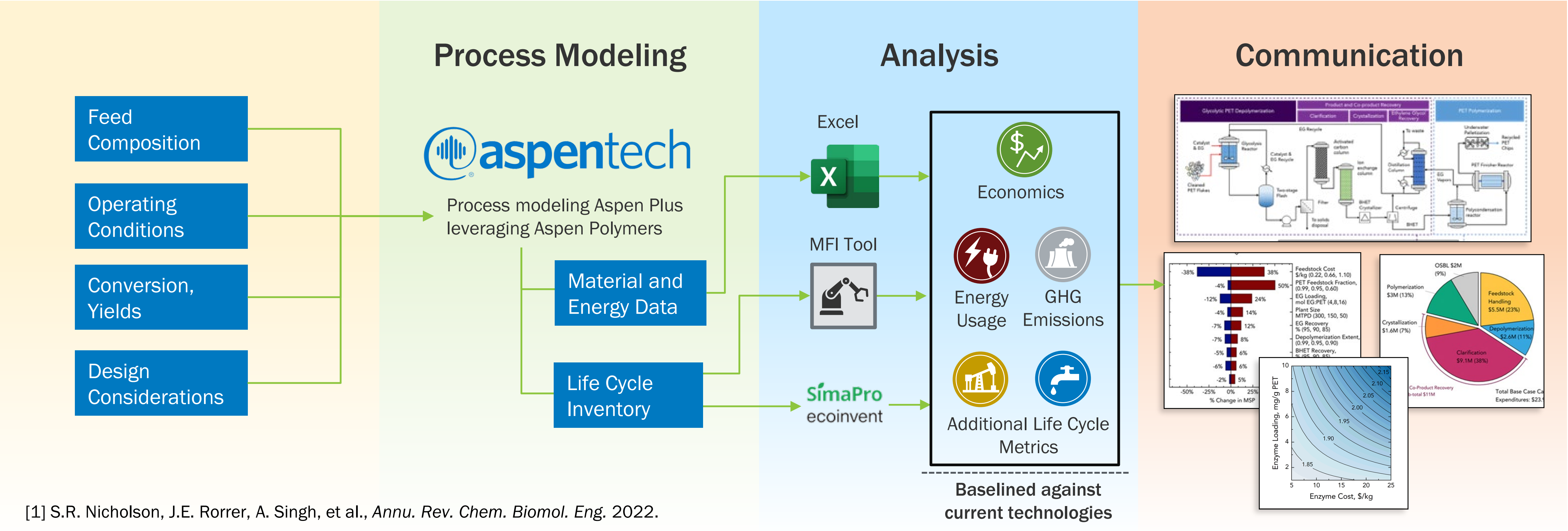


Argonne National Laboratory · Colorado State University · Los Alamos National Laboratory · MIT · NREL National Renewable Energy Laboratory · Montana State University · Oak Ridge National Laboratory · Northwestern University · SLAC National Accelerator Laboratory · University of Portsmouth

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

Approach: Analysis-guided R&D is foundational to BOTTLE

- Techno-economic analysis (TEA) and life-cycle assessment (LCA) conducted across multiple scopes
- Economics and sustainability assumptions follow **transparent** / **open-source** practices in EERE-funded R&D; framework published in recent review[1]
- Analysis is an iterative process that occurs in parallel to laboratory R&D
- Communication with each task through fortnightly team meetings and internal task meetings
- Select risks include data availability and ability to incorporate feedstock variability and quality into models



[1] S.R. Nicholson, J.E. Rorrer, A. Singh, et al., *Annu. Rev. Chem. Biomol. Eng.* 2022.

Approach: Metrics for BOTTLE projects

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:

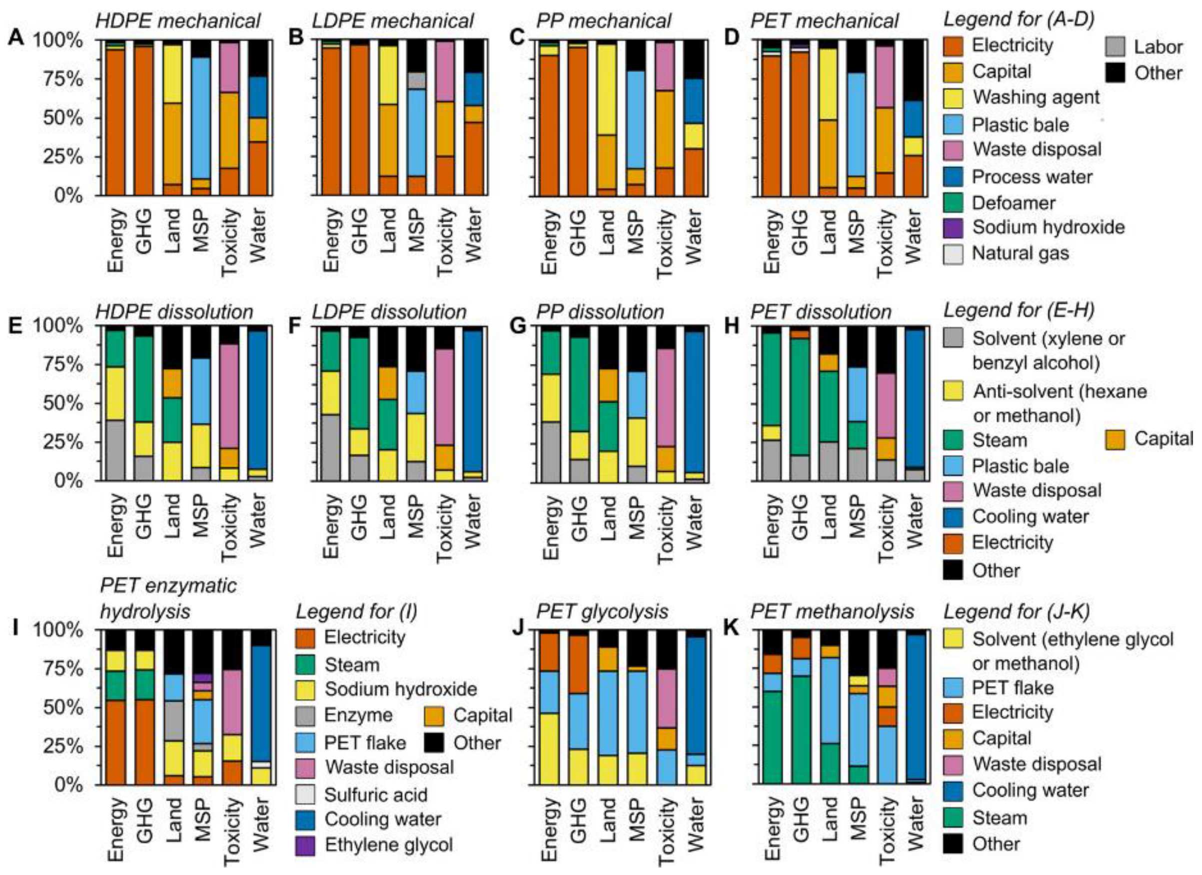
- ≥ 2x economic incentive over reclaimed materials

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]



Approach: Collaboration and communication

- <u>Centralized</u> 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

ENERGY.GOV
Office of
ENERGY EFFICIENCY & RENEWABLE ENERGY

Bioenergy Technologies Office

October 21, 2022

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

Approach: 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

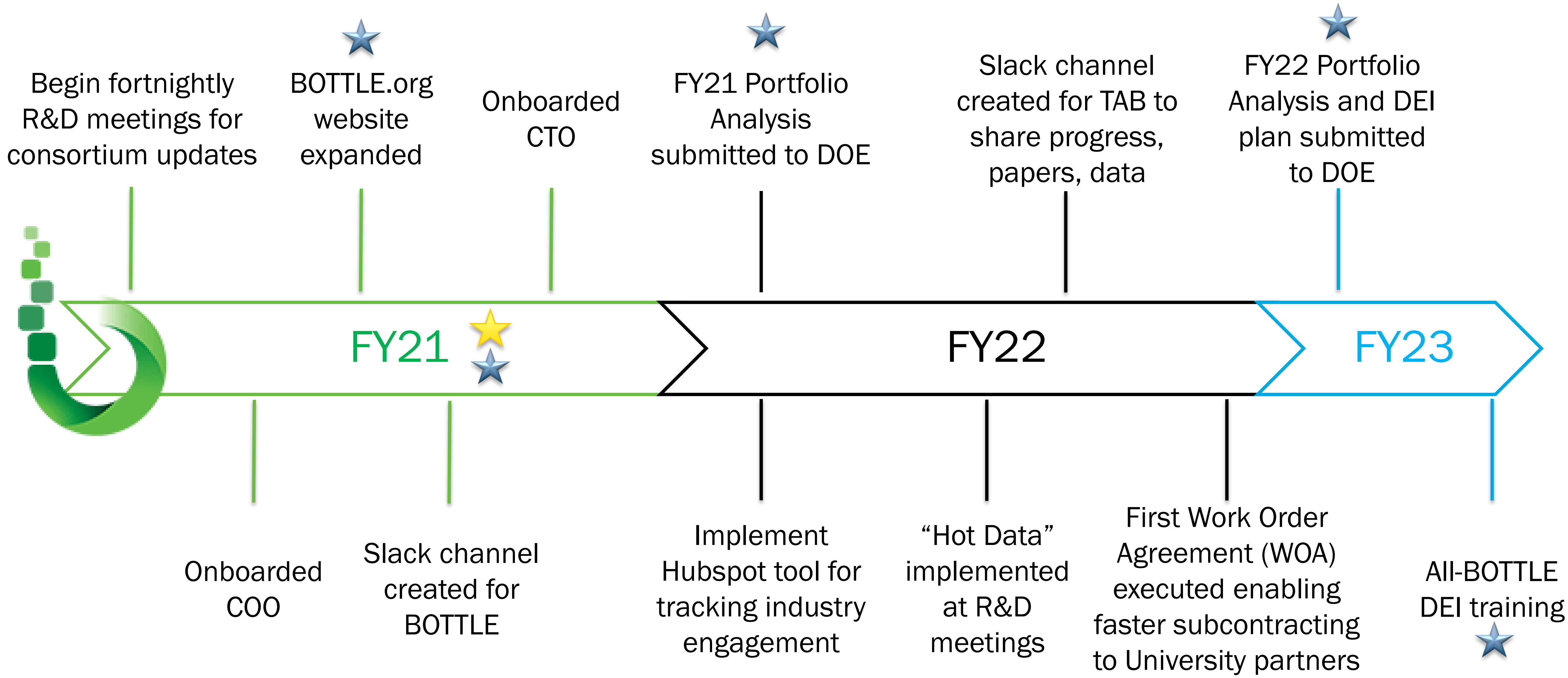
Risk: Unable to produce RBD polymers at commodity prices and achieve >50% energy savings relative to today’s materials

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

Results and achievements: BOTTLE operations

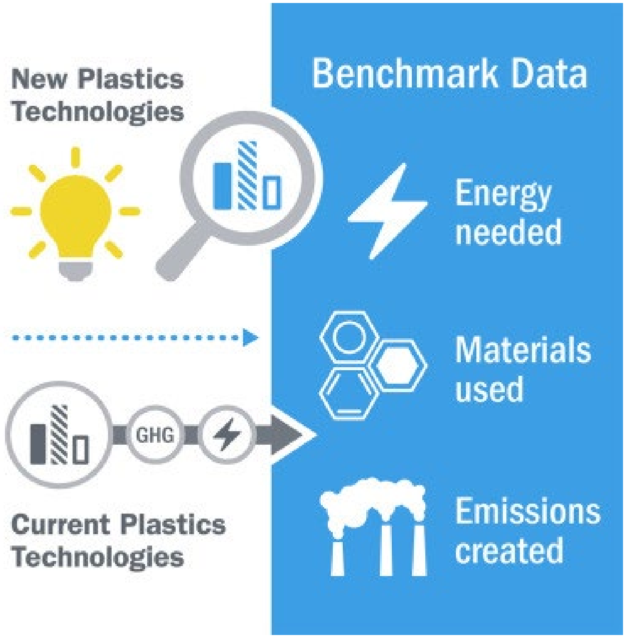


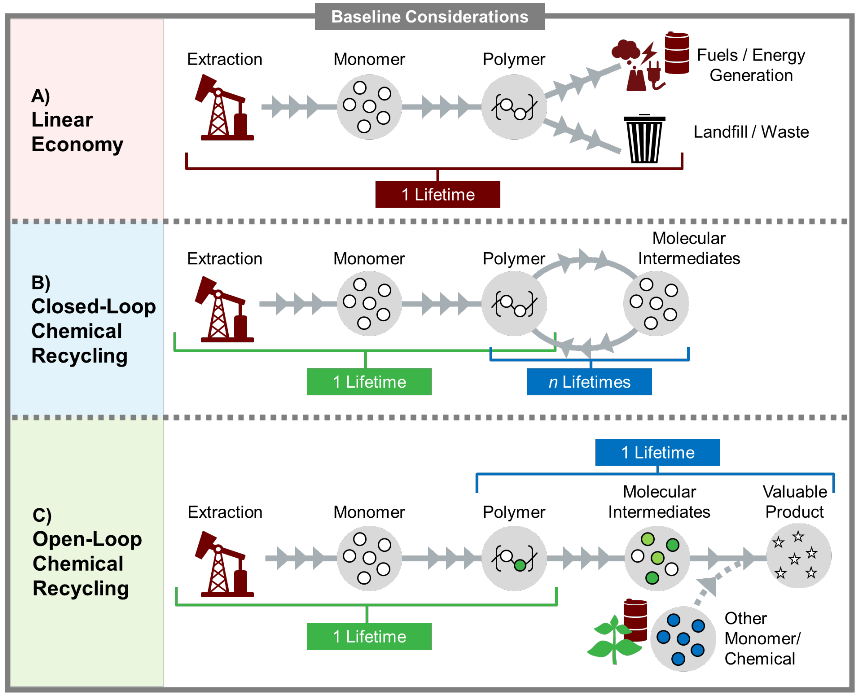
First industry partnership signed

Activity achieved a key BOTTLE milestone

Results and achievements

- Benchmarked metrics for virgin plastic production[1]
- Established analysis framework for evaluating recycling technologies[2]
- Evaluated new and existing plastic technologies



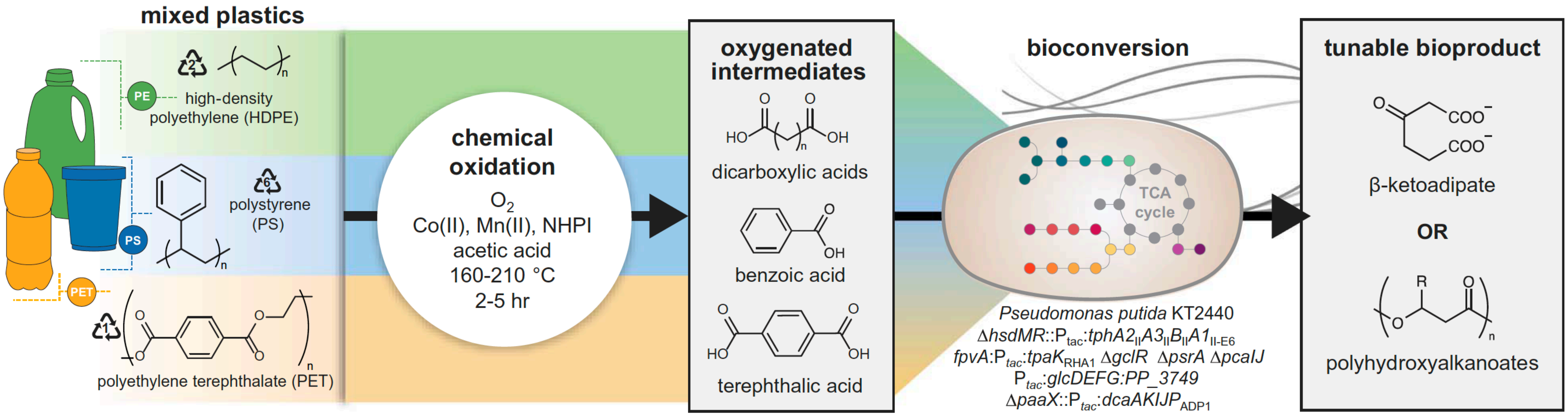


- ✓ Baseline analyses published or in peer review for:
  - ✓ PET deconstruction,[3-6]
  - ✓ Mixed plastic pyrolysis & gasification,[7-8]
  - ✓ Mechanical recycling[6]
- ❖ Additional recycling technologies in progress
- ❖ Redesign polymer pathways in progress

[1] S.R. Nicholson, N.A. Rorrer *et al. Joule* 2021. [2] S.R. Nicholson, J.E. Rorrer, A. Singh *et al. Annu. Rev. Chem. Biomol. Eng.* 2022. [3] A. Singh *et al. Joule* 2021. [4] T. Uekert *et al. Green Chem.* 2022. [5] N.A. Rorrer *et al. in preparation* 2023. [6] T. Uekert *et al. ACS Sustain. Chem. Eng.* 2023. [7] G. Yadav *et al. in revision* at *Energy Env. Sci.* [8] S. Afzal *et al. in revision* at *Green Chem.*

Results and achievements

Mixed plastics waste valorization through tandem chemical oxidation and biological funneling



Goal: depolymerize mixed plastics waste to bio-available oxygenates with robust process

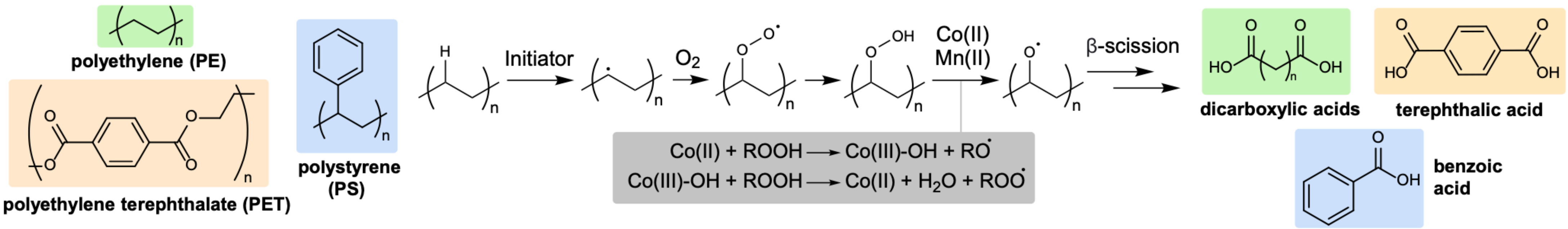
Background: catalysis has precedent in the industrial process to produce terephthalic acid

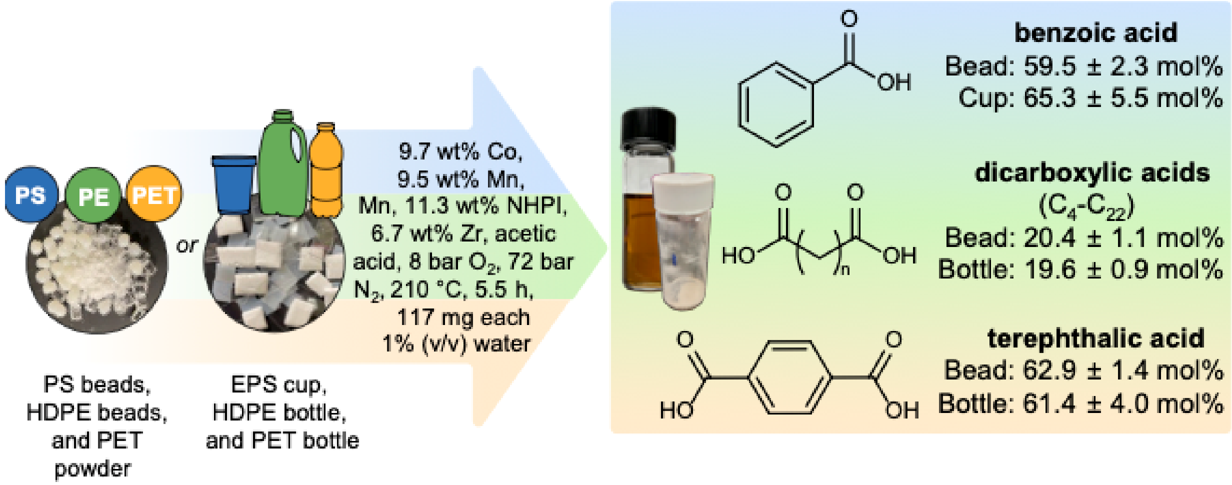
Impact: strategy is tolerant of contaminants in mixed plastics waste including PVC, dyes, etc.

Future work: offers a direct route to produce designer building blocks (with Upcycling and Redesign)

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

Results and achievements

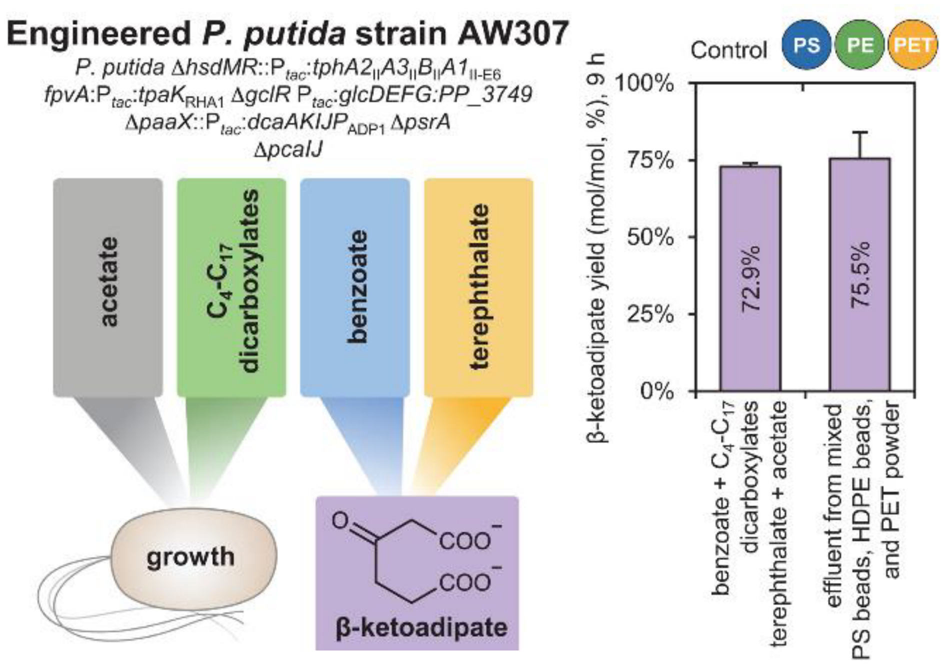




Mixed plastics can be simultaneously deconstructed…

Impact: Spun out a company from BOTTLE (Tereform)

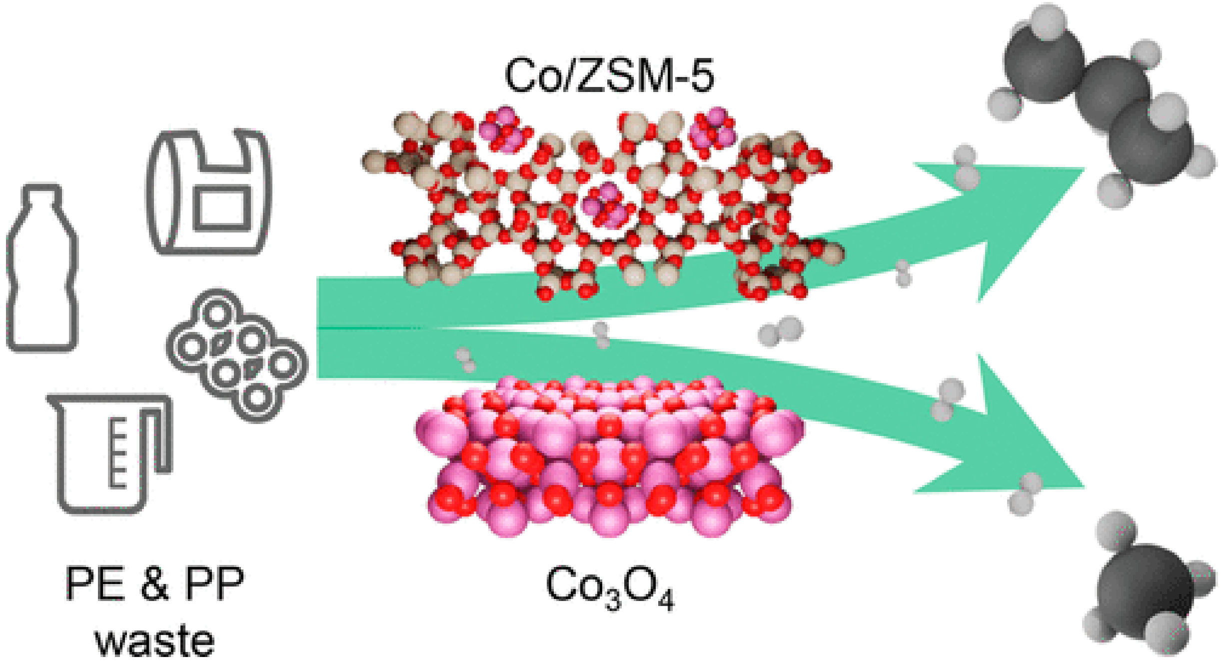
…and converted to a single product

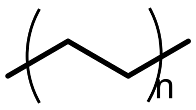


Sullivan, Werner, Ramirez, Ellis *et al.*, *Science* 2022

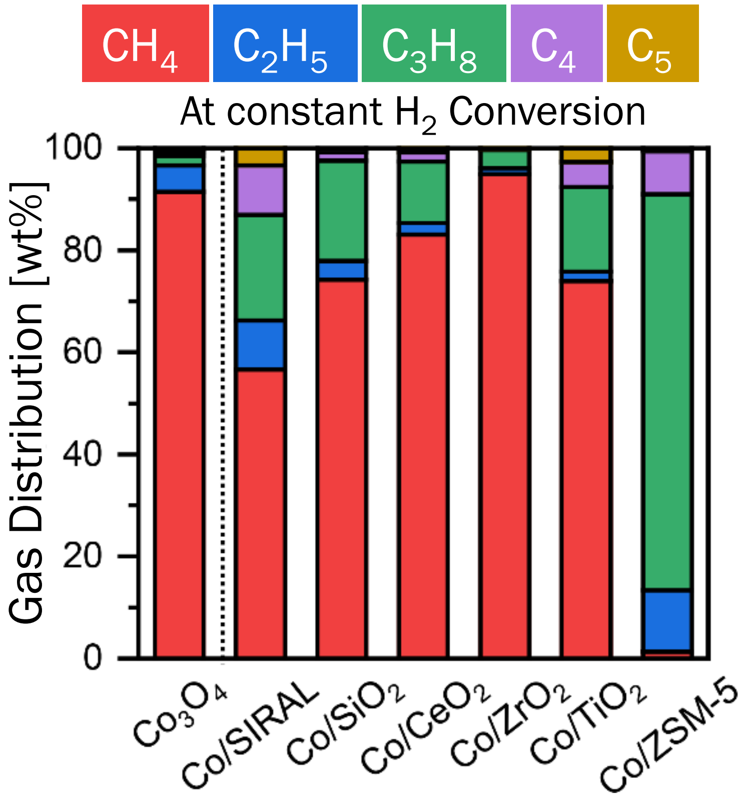
Results and achievements

Hydrogenolysis of polyethylene and polypropylene into propane over cobalt-based catalysts





250°C, 40 bar H_2, 20 h,
600 RPM, 50 $mg_{eq,Co}$
catalyst (5 wt% Co)

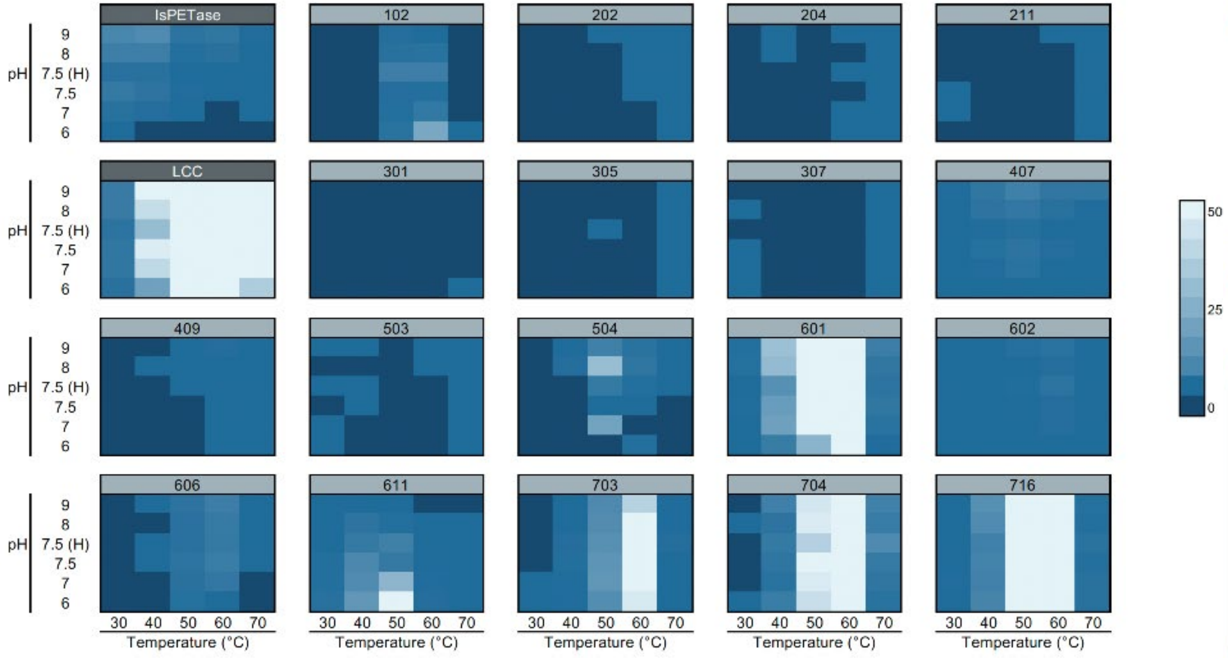


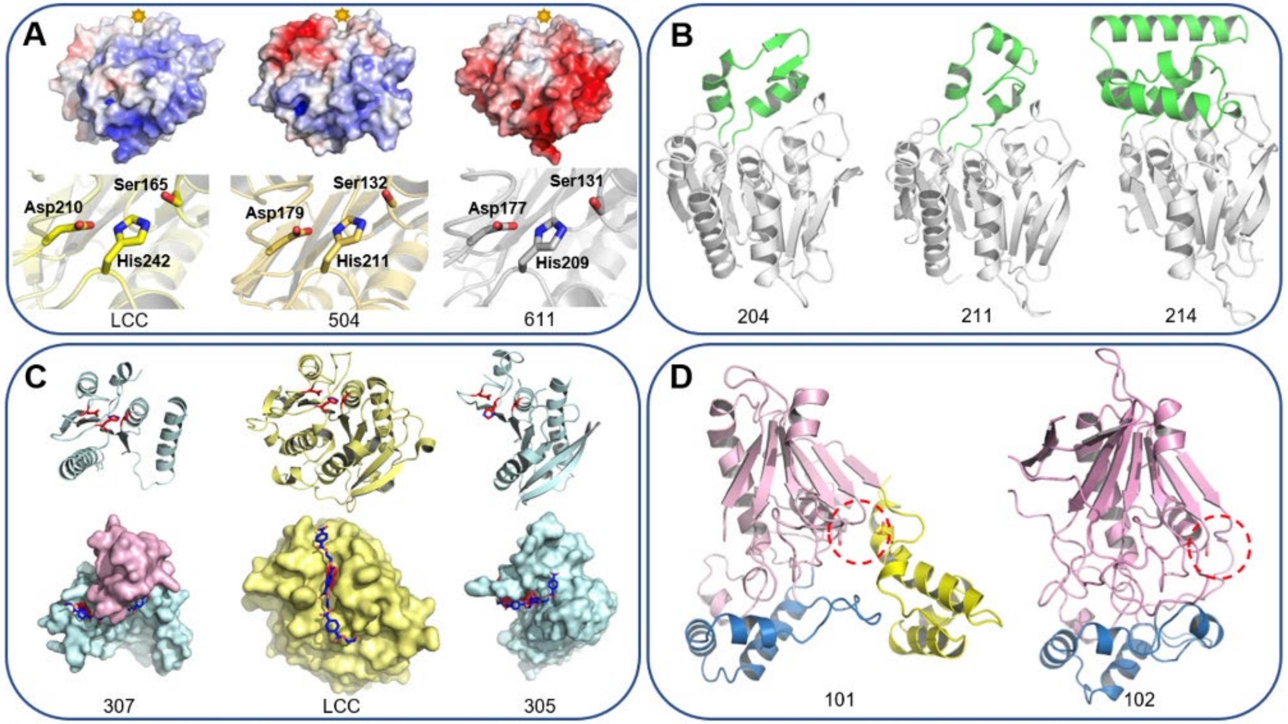
Mixed PE and PP can be converted at moderate conditions to a single product

Zichittella *et al.*, *JACS Au* 2022

Results and achievements

Sourcing thermotolerant poly(ethylene terephthalate) hydrolase scaffolds from natural diversity





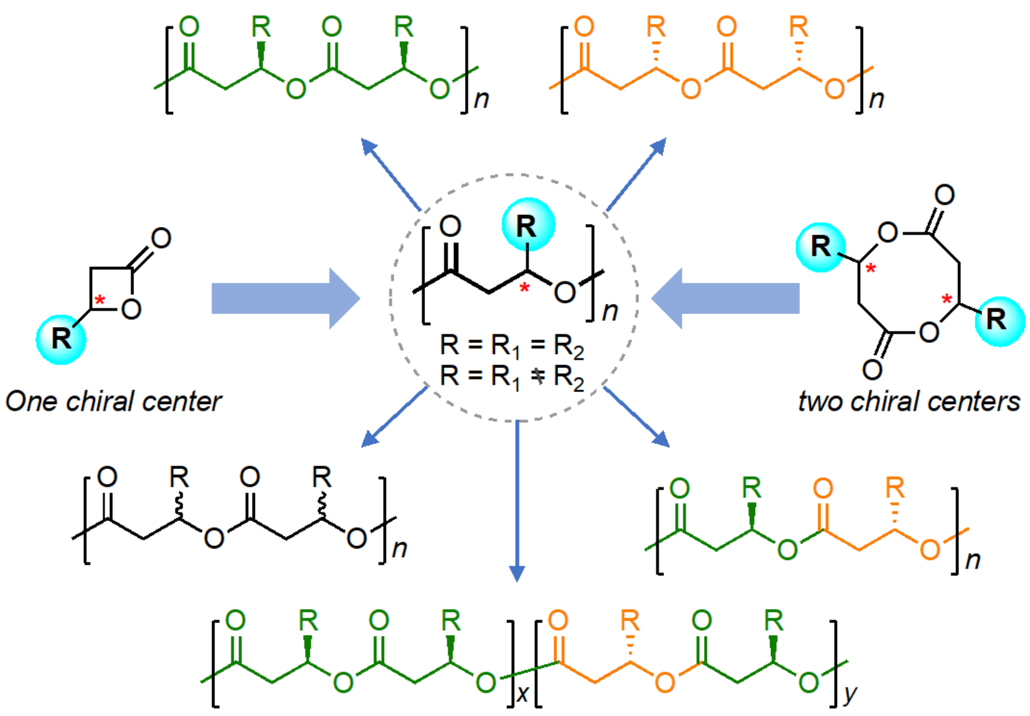
Outcome: Discovered first enzyme with preferential activity towards crystalline PET

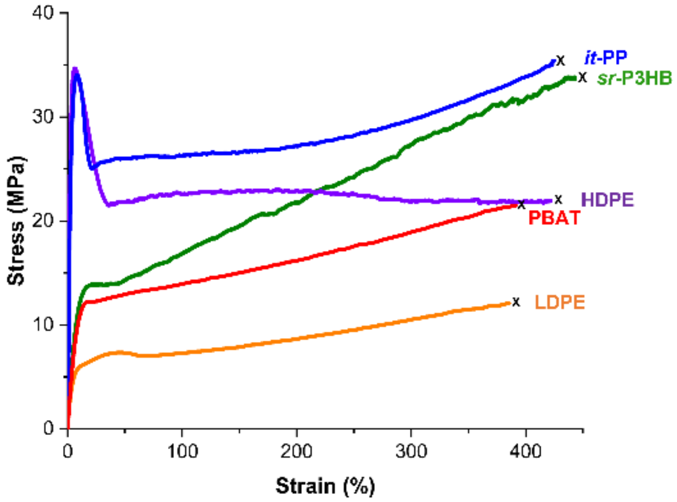
Impact: Enzymes with activity on crystalline PET could reduce the pretreatment energy consumption and associated GHG emissions

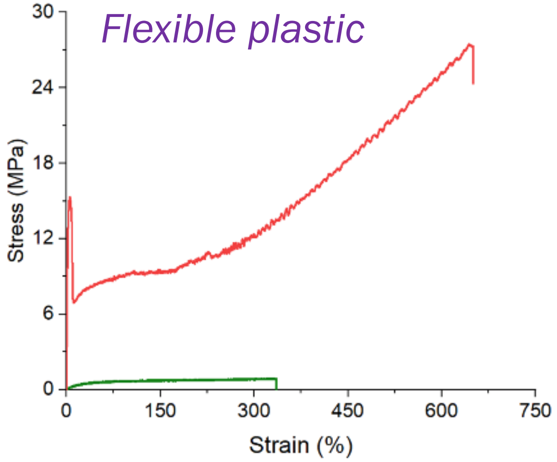
Ongoing work: Newly discovered enzymes are going through directed evolution pipeline

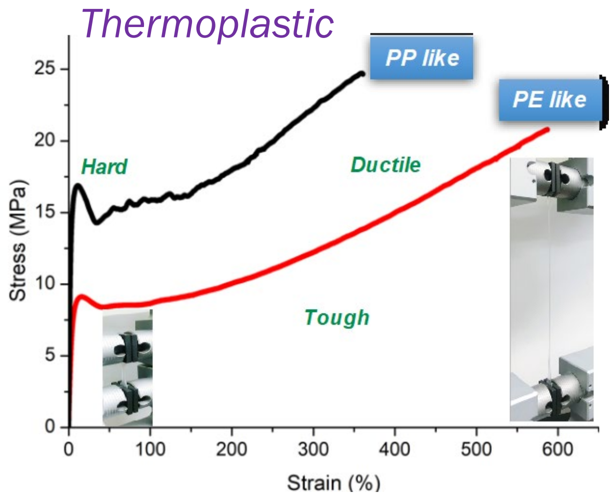
Erickson, Gado, *et al.*, *Nature Comm.* 2022

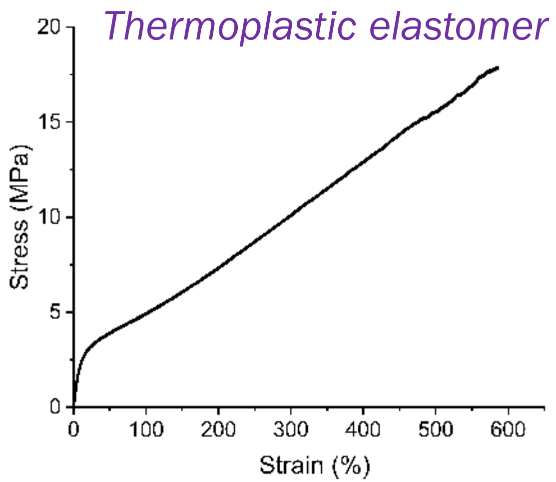
Results and achievements









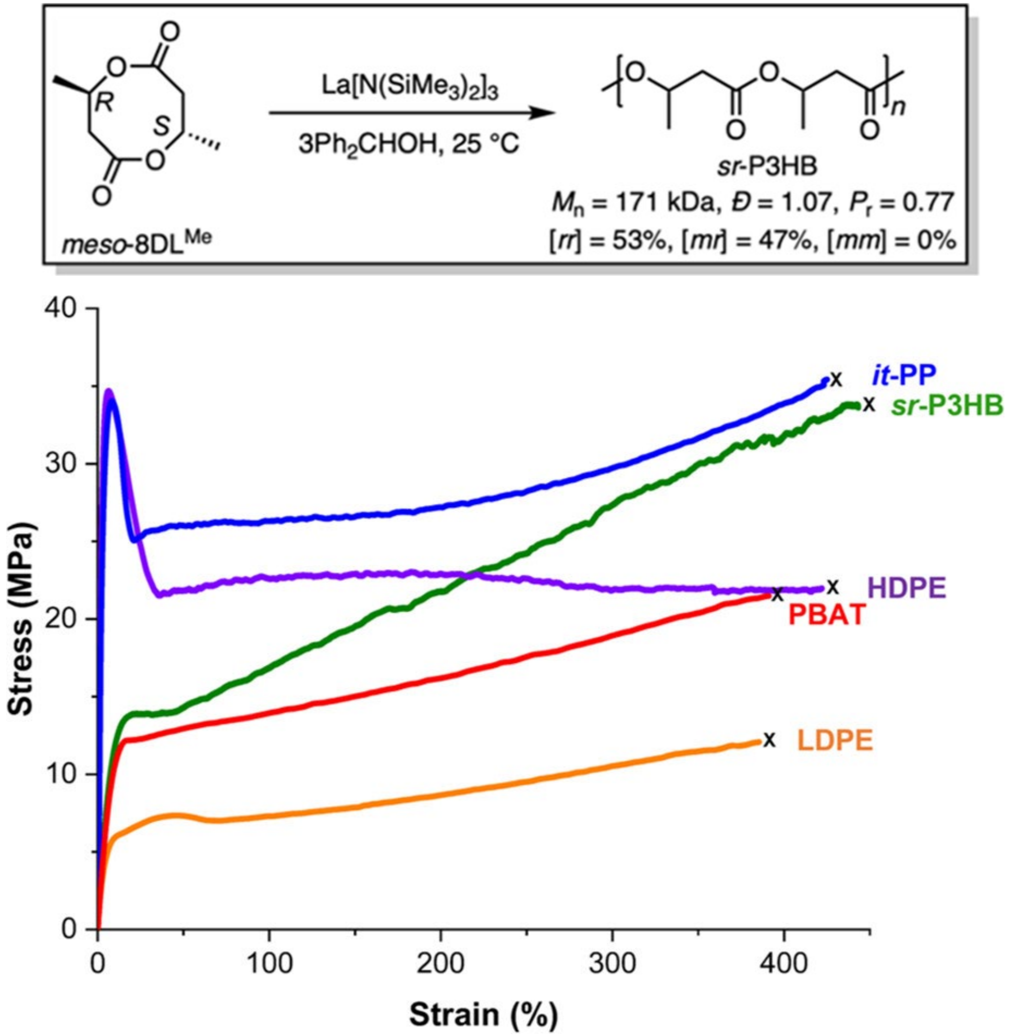


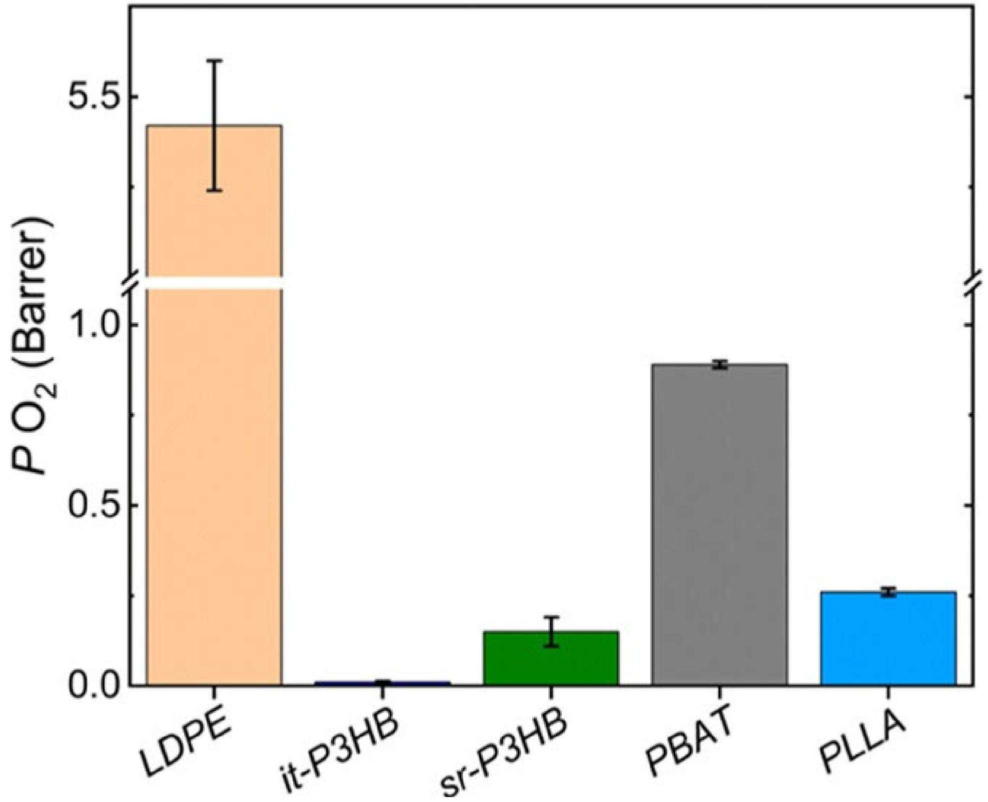
- Fast kinetics in synthesis (minutes to hours)
- Scalability and large scope of monomers
- Designer PHAs with properties of all polymer classes
- Promising alternatives to LDPE, HDPE, PP, etc.

Westlie *et al. Prog. Polym. Sci.* 2022

Results and achievements

Installing controlled stereo-defects yields semicrystalline and biodegradable poly(3-hydroxybutyrate) with high toughness and optical clarity

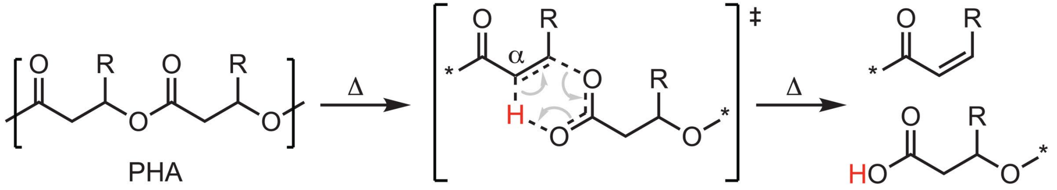




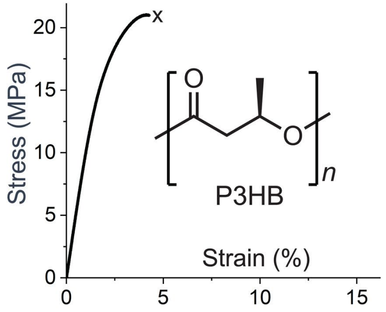
Quinn, Zhang *et al.*, *JACS* 2023

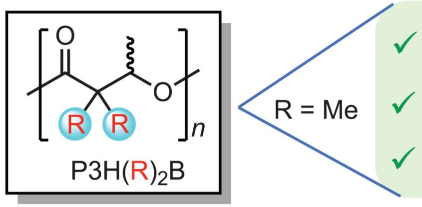
Results and achievements

Chemically circular, mechanically tough, and melt-processable polyhydroxyalkanoates

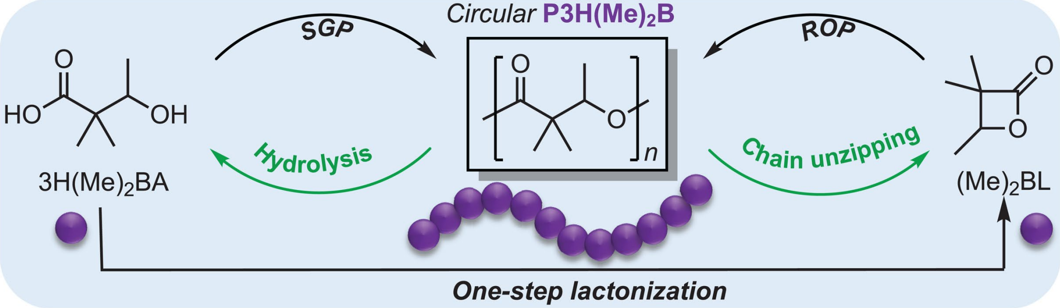


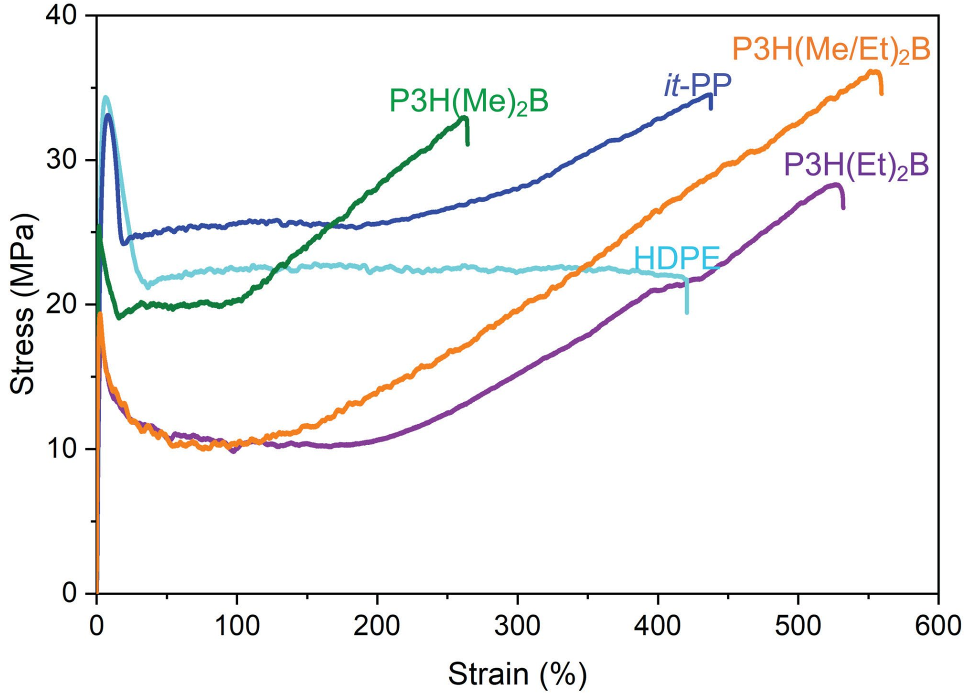
- Not melt-processable (T_d ~250 °C)
- Mechanically brittle (ε_b ~4% for *it*-P3HB)
- Not chemically recyclable (to monomer)





- ✓ Melt-processable (T_d up to 335 °C)
- ✓ Crystalline yet ductile (ε_b >200%)
- ✓ Recyclable (to monomer)



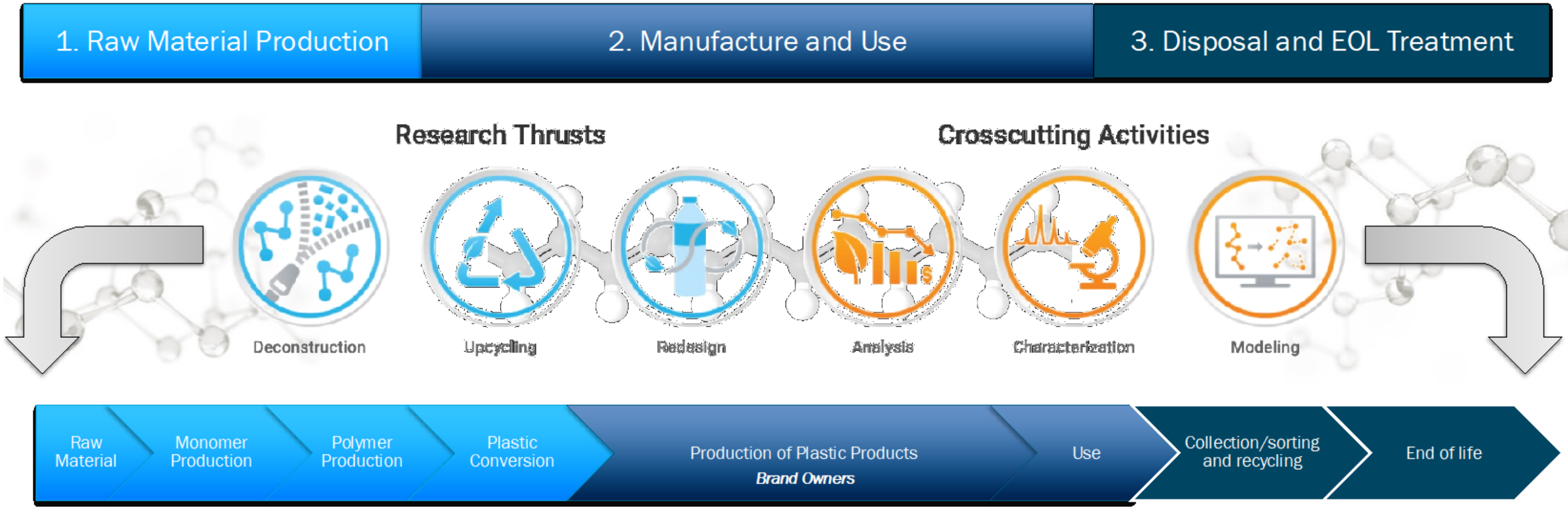


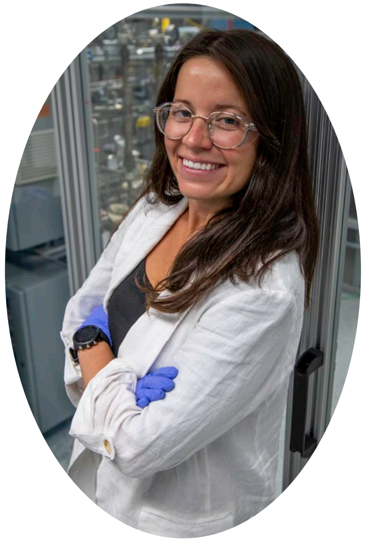
Zhou, Zhang, Shi *et al.*, *Science* 2023

Results and achievements

BOTTLE's industry engagement history:

- BOTTLE created a centralized business development (BD) platform and focused BD effort
- Created a dedicated BD/research role (Chief Technology Officer) to streamline engagement and lead CRADA projects
- Onboarded BD tools to streamline BOTTLE engagement pipeline (Hubspot)
- Leveraged AOP-funded BOTTLE innovations portfolio to design projects with near-term industrial relevance
- Identified companies to target for collaboration using an industry landscape analysis and external consulting report
  - Initial traction with brand owners





BOTTLE CTO
Kat Knauer

BOTTLE's industry engagement goals:

- Solve real-world problems in plastics upcycling via targeted, company-funded projects
- Promote industrial engagement via streamlined access to BOTTLE partners and technologies
- Act as a supply chain navigator and collaborate with companies to scale and deploy BOTTLE technologies into the U.S. economy

amazon – Deconstruction & redesign of polyesters

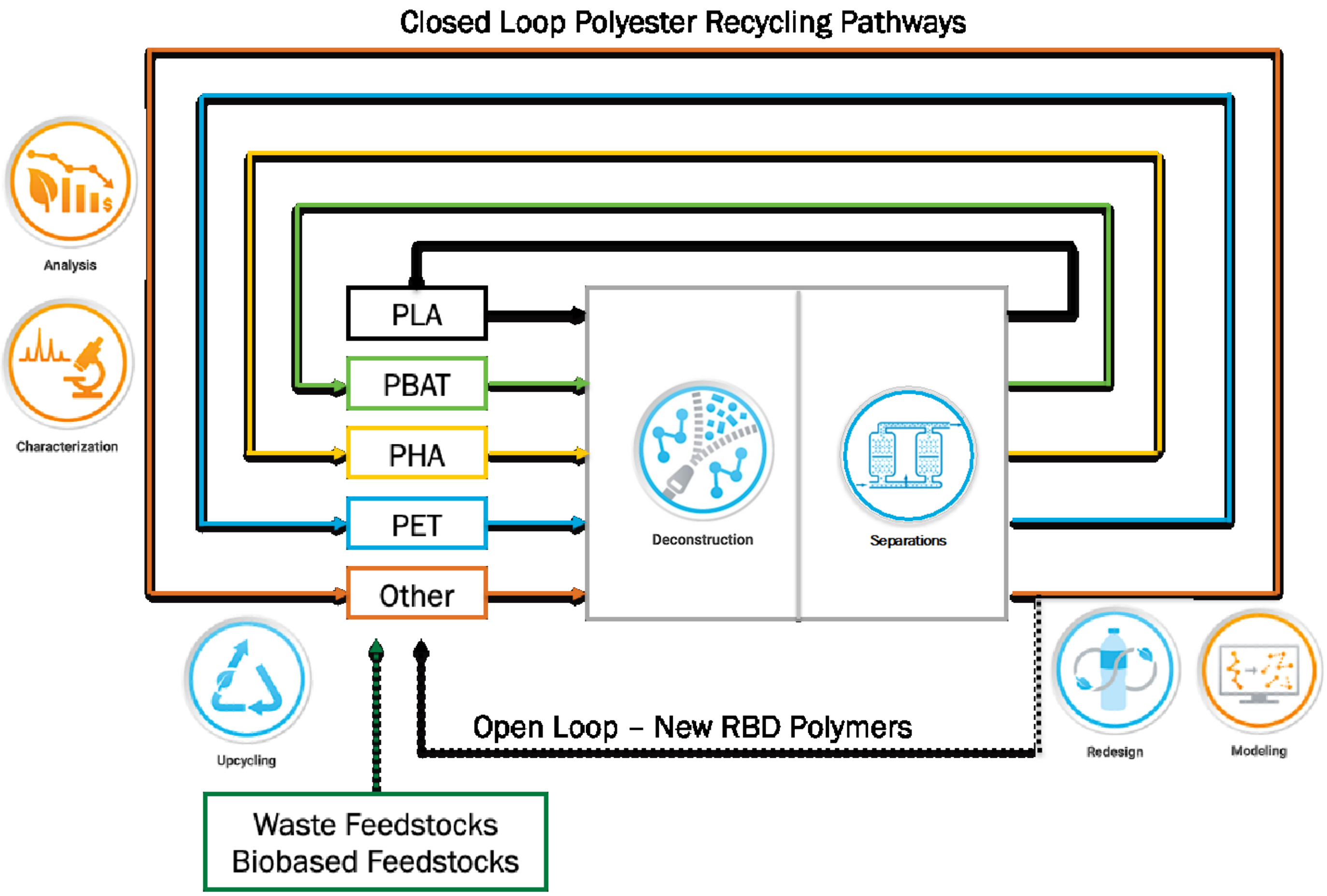
Overall goals:
- Develop a closed-loop, integrated recycling technology for mixed polyesters
- Develop a recycle-by-design and biodegradable PE alternative

Team size:
- >15 BOTTLE researchers

BOTTLE participants:
- CSU, NREL, SLAC

BOTTLE tasks:
- Deconstruction, Upcycling, Redesign, Characterization, and Analysis

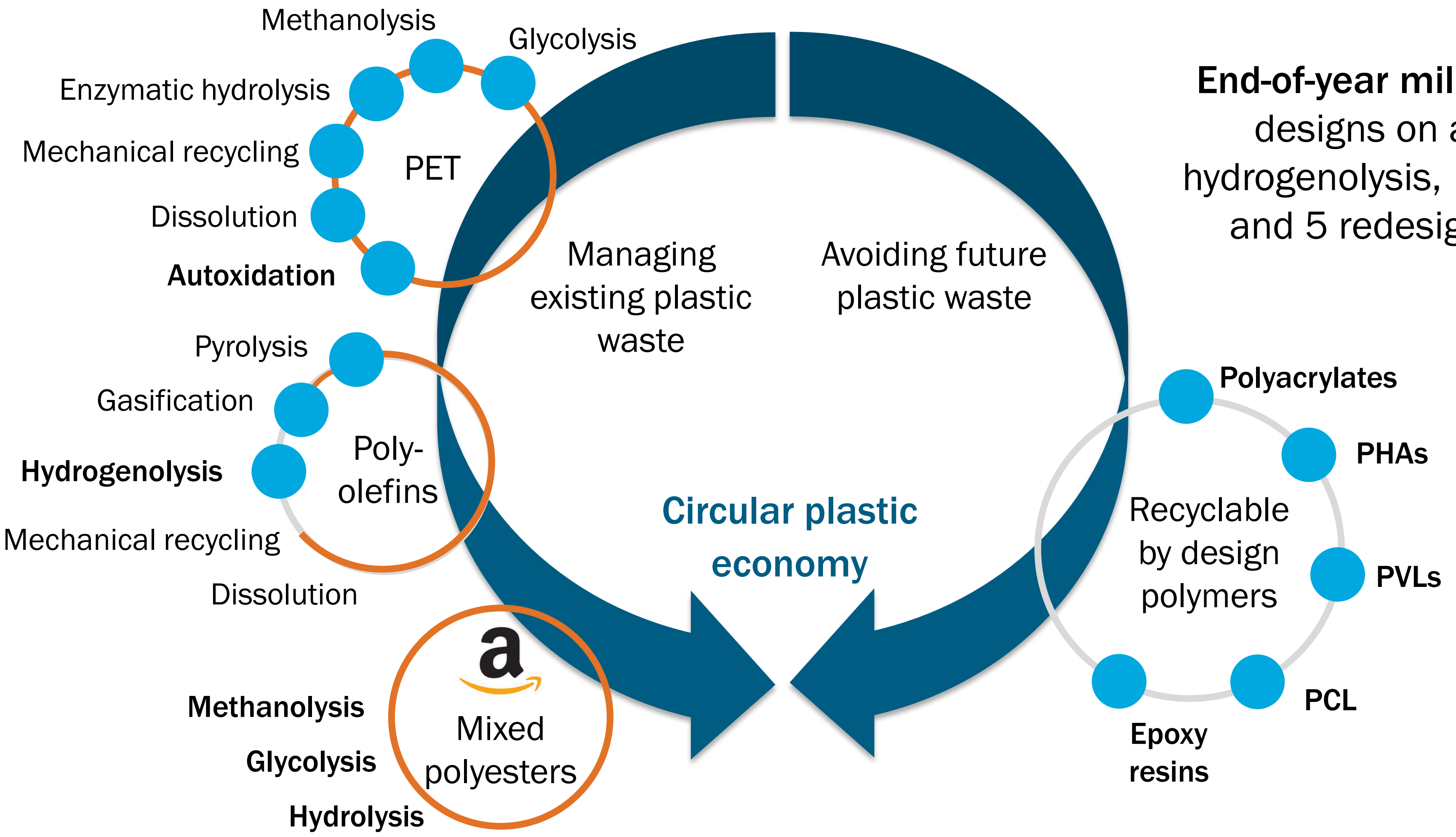
BETO investment leveraged:
- PET deconstruction technologies[1-3]
- TEA/LCA data on PET deconstruction[4-5]
- Designer PHA portfolio[5-8]



[1]Nicholson, Rorrer *et al. Joule* 2019; [2]Knott, Erickson *et al. PNAS* 2020; [3]Werner *et al. Met Eng.* 2021; [4]Singh *et al. Joule* 2021; [5]Uekert *et al. Green Chem.* 2022; [6]Tang et al. *Nat. Commun.* 2018; [7]Tang et al. *Science* 2019; [8]Tang et al. *Angew. Chem.* 2020

Future work, technology transfer, and impact

Finalized and upcoming analyses



End-of-year milestones: Deliver designs on autoxidation, hydrogenolysis, PET conversions, and 5 redesigned polymers

= stand-alone case study = comparative analysis = plastic family

Acronyms: polyhydroxyalkanoates (PHAs), polyvalerolactones (PVLs), polycaprolactone (PCL)

Future work, technology transfer, and impact

Industrial impact:

- >40 BOTTLE researchers on industry projects
- >150 Industrial partners engaged
- 31 Patent applications (5 CRADA subject inventions)
- 7 Industrial CRADAs executed
- 3 FOA CRADAs executed and started
- 2 Industrial CRADAs in contracting
- 2 BOTTLE spin-off companies: Tereform & Eco Polymers

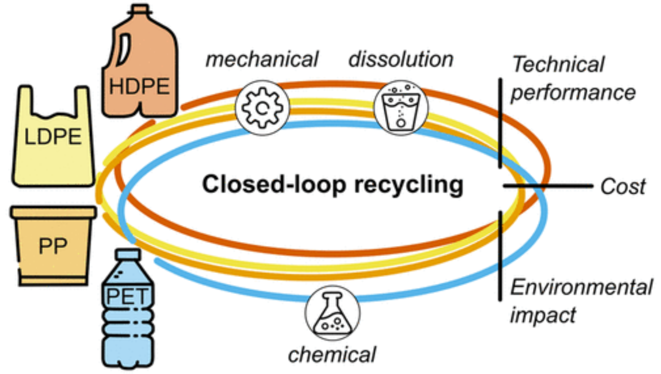
Large companies → CRADAs

Mid/small co. and startups → FOAs, DOE funded incubators

Future work, technology transfer, and impact

Overall impact:

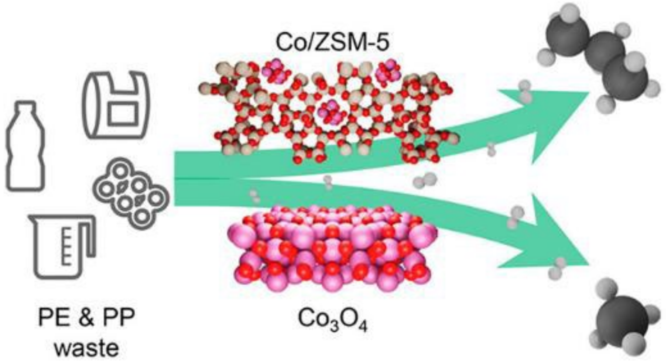
- Developed framework for circularity analysis – attracting engagement from industry, NGOs, and academic partners
- Substrate characterization methods proposed for scientific reproducibility (Ellis *et al., Nature Catal.* 2021)
- Training next-generation leaders in polymer sustainability and conducting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



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

Resulted in:

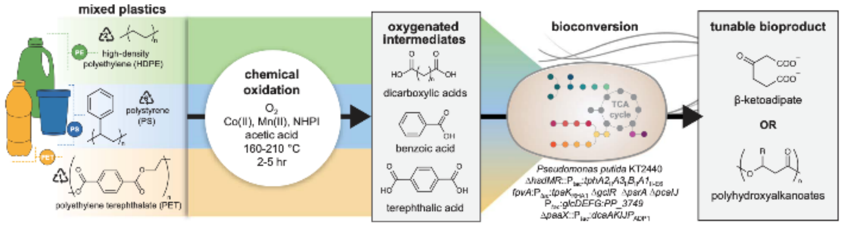
- 4+ industrial contacts
- 32 news outlets



Zichittella *et al., JACS AU* 2023

Resulted in:

- 2+ industrial contacts
- 31 news outlets



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

Resulted in:

- 10+ industrial contacts
- 80 news outlets

Thank you!

Argonne National Laboratory

Meltem Urgun-Demirtas
Chaoyi Ba
Thai Scheve
Reni Truhtcheva - *Owikoti*
Shu Xu
Haoran Wu

Colorado State University

Eugene Chen
Deepak Barange
Ryan Clarke
Robin Cywar
Maëlle Gace
Reid Gilsdorf
Ravikumar Gowda
Celine Parker
Ethan Quinn
Eswara Rao
Ainara Sangroniz
Changxia Shi
Andrea Westlie
Zhen Zhang
Li Zhou

Los Alamos National Laboratory

Taraka Dale
Shounak Banerjee
Carson Gido
Rommel Granja
Tom Groseclose
Ramesh Jha
Erin Kober
Hau Nguyen
Sang-Min Shin

MIT

Yuriy Román
Lucas Baston
Anna Brenner
Griffin Drake
Alexi Khechfe
Ydna Questell
Julie Rorrer
Clara Troyano-Valls
Xiao Wang
Bing Yan
Guido Zichitella

Montana State University

Jen DuBois
Emmanuel Akpoto
Jessica Lusty Beech
Rita Clare
Dongjin Kim
Will Kincannon
Ronivaldo Rodrigues da Silva
Ari Romberg
Monica Sanchez

Northwestern University

Linda Broadbelt
Sri Bala Gorugantu
Sai Phani Kumar Vangala
Joseph Ni
Alexander Shaw
Quan Zhang
William Sprague
Kevin Shebek

NREL – National Renewable Energy Laboratory

Gregg Beckham
Bob Allen
Hannah Alt
Abhay Athaley
Robert Baldwin
David Brandner
Jeremy Bussard
Birdie Carpenter
Young-Saeng Cho
Kathy Cisar
Amy Cuthbertson
Mackenzie Denton
Jason DesVeaux
Bryon Donohoe
Meredith Doyle
Lucas Ellis
Japheth Gado
Oliver Greener
Stefan Haugen
Laura Hollingsworth
Morgan Ingraham
Katrina Knauer
Megan Krysiak
Eugene Kuatsjah
Ciaran Lahive
Clarissa Lincoln
Swarnalatha Mailaram
William Michener
Joel Miscall
Hyunjin Moon
Ana Morais
Brenna Norton-Baker
Eric Payne
Kelsey Ramirez
Michelle Reed
Erik Rognerud
Nic Rorrer
Ron Schoon
Lisa Stanley
Kevin Sullivan
Taylor Uekert
Allison Werner
Sean Woodworth
Geetanjali Yadav
Shaik Afzal
Brenna Black
Bonnie Buss
Erika Erickson
Mikhail Konev
Scott Nicholson
Avantika Singh
Nolan Wilson

U.S. Department of Energy – Office of Energy Efficiency & Renewable Energy
Bioenergy Technologies Office
Advanced Materials & Manufacturing Technologies Office

Coralie Backlund, BETO
Gayle Bentley, BETO
Jay Fitzgerald, BETO
Kate Peretti, AMMTO
Michelle Seitz, AMMTO

Oak Ridge National Laboratory

Adam Guss
Bill Alexander
Austin Carroll
Carrie Eckert
Jim Elkins
Rich Giannone
Bob Hettich
Jay Huenemann
Ikenna Okekeogbu
Darren Parker
Sirisha Parimi
Miriam Silberman
Shanice Taylor
Jessie Tweedie
Walter Woodside

BOTTLE – changing the way we recycle – U.S. Department of Energy

Technical Advisory Board

Tim Long
Thomas Epps
Scott Farling
Adrienne Huston-Davenport
Guy Joly
Kara Lavender Law
Susannah Scott
Brent Shanks
Margaret Sobkowicz-Klein
Mark Spalding
Scott Trenor

SLAC National Accelerator Laboratory

Chris Tassone
Arun Asundi
Simon Bare
Amani Ebrahim
Sarah Hesse
Anjani Maurya
Riti Sarangi
Chris Takacs
Yue Wu

University of Portsmouth

Andy Pickford
Victoria Bemmer
Anastasia Callaghan
Simon Cragg
Rosie Graham
John McGeehan
Rory Miles
Joy Watts
Luisana Avilan
Paul Cox
Raj Gill
Gerhard Konig
Bruce Lichtenstein
Michael Zahn

Questions?

BOTTLE Consortium | AMMTO

Gregg T. Beckham, NREL, gregg.beckham@nrel.gov