bottle

changing the way we recycle

U.S. DEPARTMENT OF ENERGY

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

DOE Bioenergy Technologies Office (BETO) 2023 Project Peer Review

BOTTLE 7 – Industry Projects & Engagement

April 3, 2023

Technology Session Review Area: Plastics Deconstruction and Redesign

PI: Katrina Knauer, BOTTLE CTO, National Renewable Energy Laboratory

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BIOENERGY TECHNOLOGIES OFFICE
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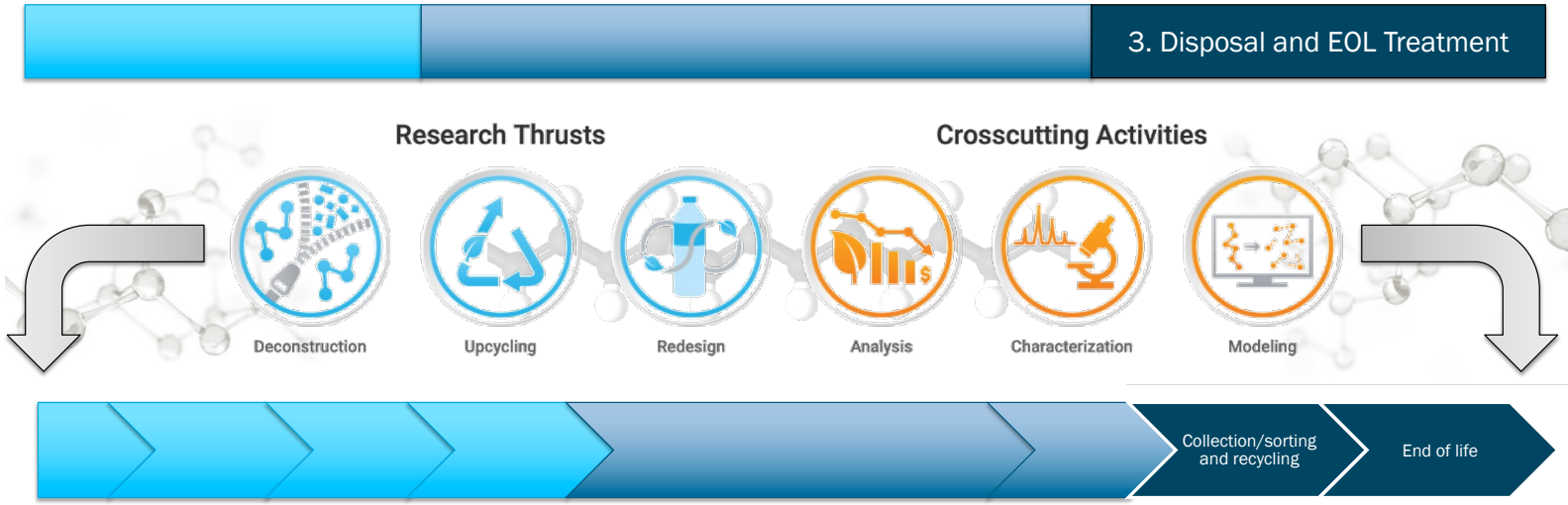
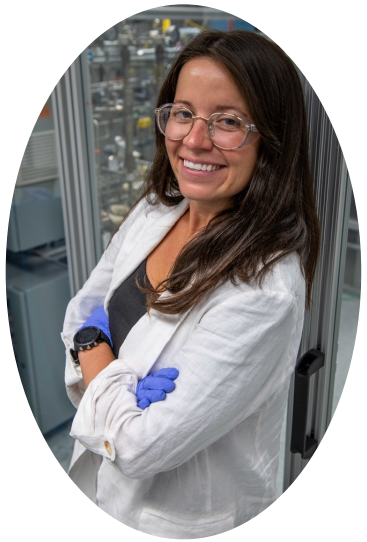
Overview – BOTTLE industry engagement

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

BOTTLE Industry Engagement Approach

- Intro to BOTTLE and flagship projects
- Solicit challenges from companies
- Company shares key sustainability metrics

- Outline a scope of work (TRL 2-3)
- Initial tasks are usually 6-18 months (hiring for short projects can be challenging)
- Format funding as stage-gate approach

Set up meeting

Establish NDA

Brainstorming

Iteration & Negotiation

Stage 0: Prospecting → **Stage 1: Initial Engagement** → **Stage 2: Knowledge Sharing** → **Stage 3-4: Proposal & Contracting** → **Stage 5: Opportunity Won**

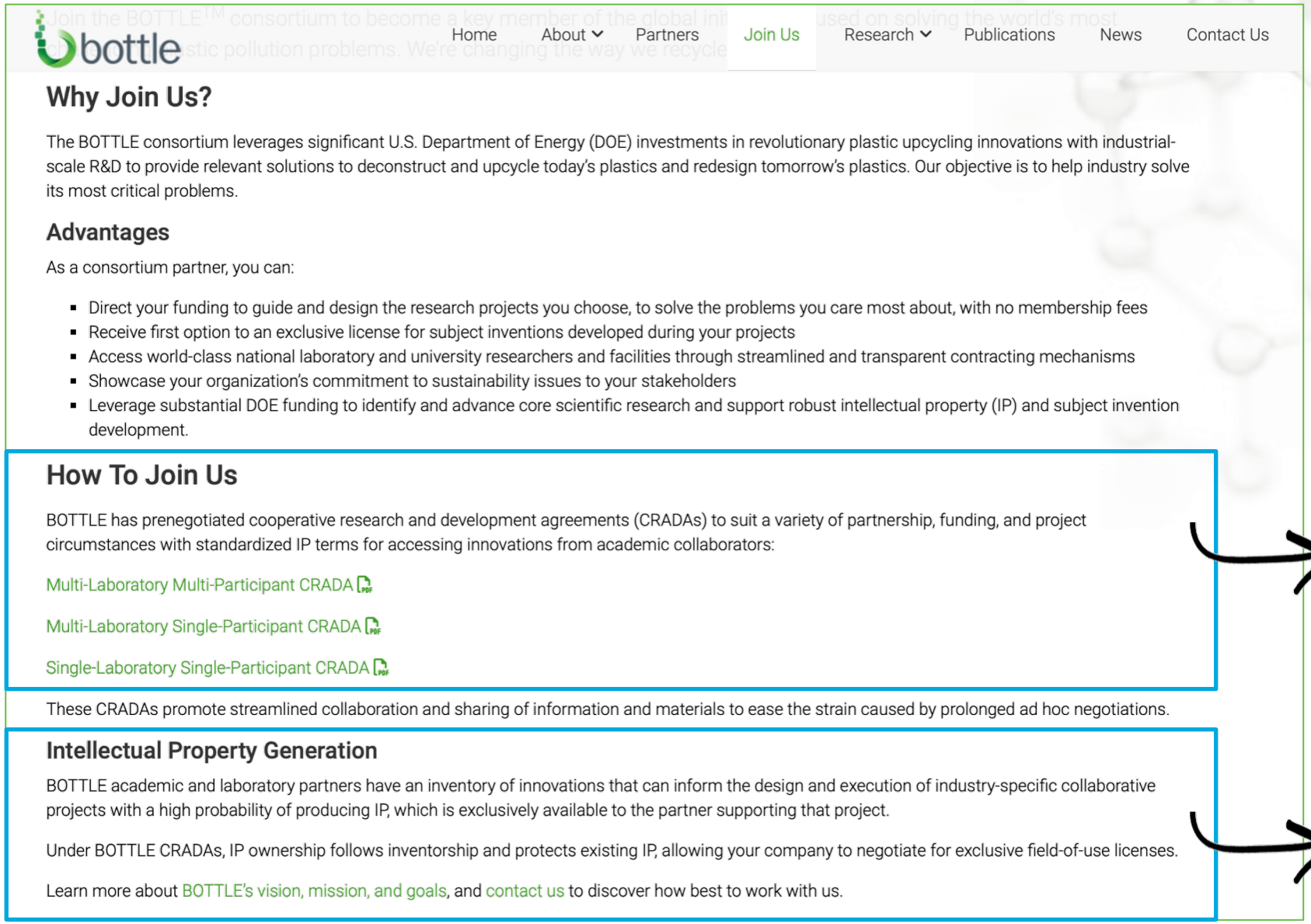
- Conferences
- Networking
- Market reports
- Publications and patents

- Share BOTTLE capabilities and strategies
- Show line-of-sight to scale
- Preliminary TEA/LCA helps guide discussions
- Company also shares data/previous work

- Update project managers on kickoff and milestone dates
- Update subcontracting agreements for funds transfers to BOTTLE partners

Blue text – Key learnings since FY21 peer review *Red text – Key challenges*

Documents on BOTTLE website help accelerate contracting



BOTTLE CRADA templates available on website

IP management plan signed by all BOTTLE institutions

Progress and outcomes BOTTLE industry engagement

6 Executed industry CRADAs since FY21
8 Successful go/no-go meetings
2 CRADA extensions and follow-on funding

4 CRADA projects currently in contracting

Gaining traction with multiple players in plastic supply chain beyond brand owners

Expanding model to include philanthropic/VC groups

Company projects include deconstruction, upcycling, and redesign of plastics

Note: Logos omitted for proprietary partners

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:

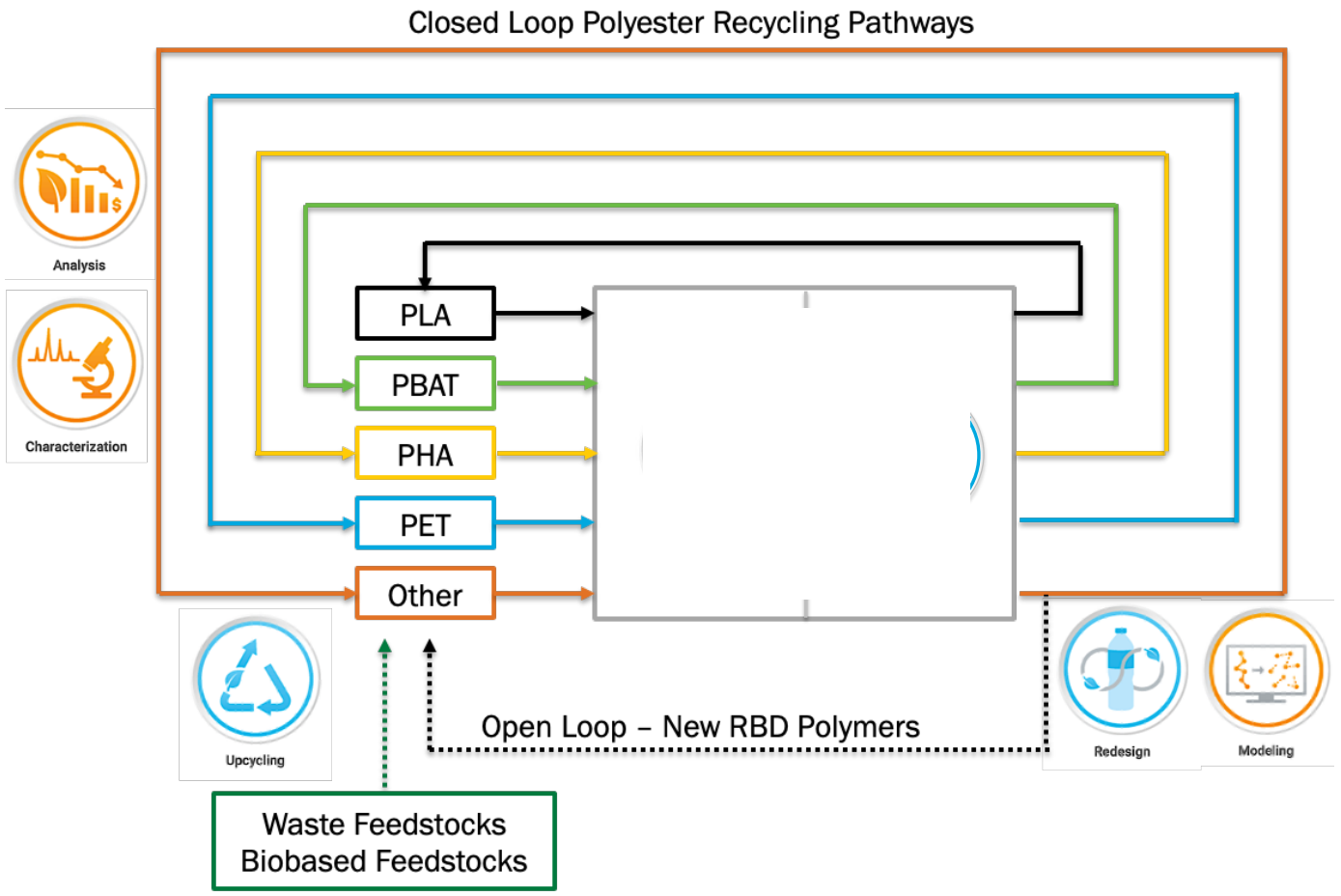
- CSU, NREL, SLAC

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

KraftHeinz – Redesign of food packaging for end-of-life

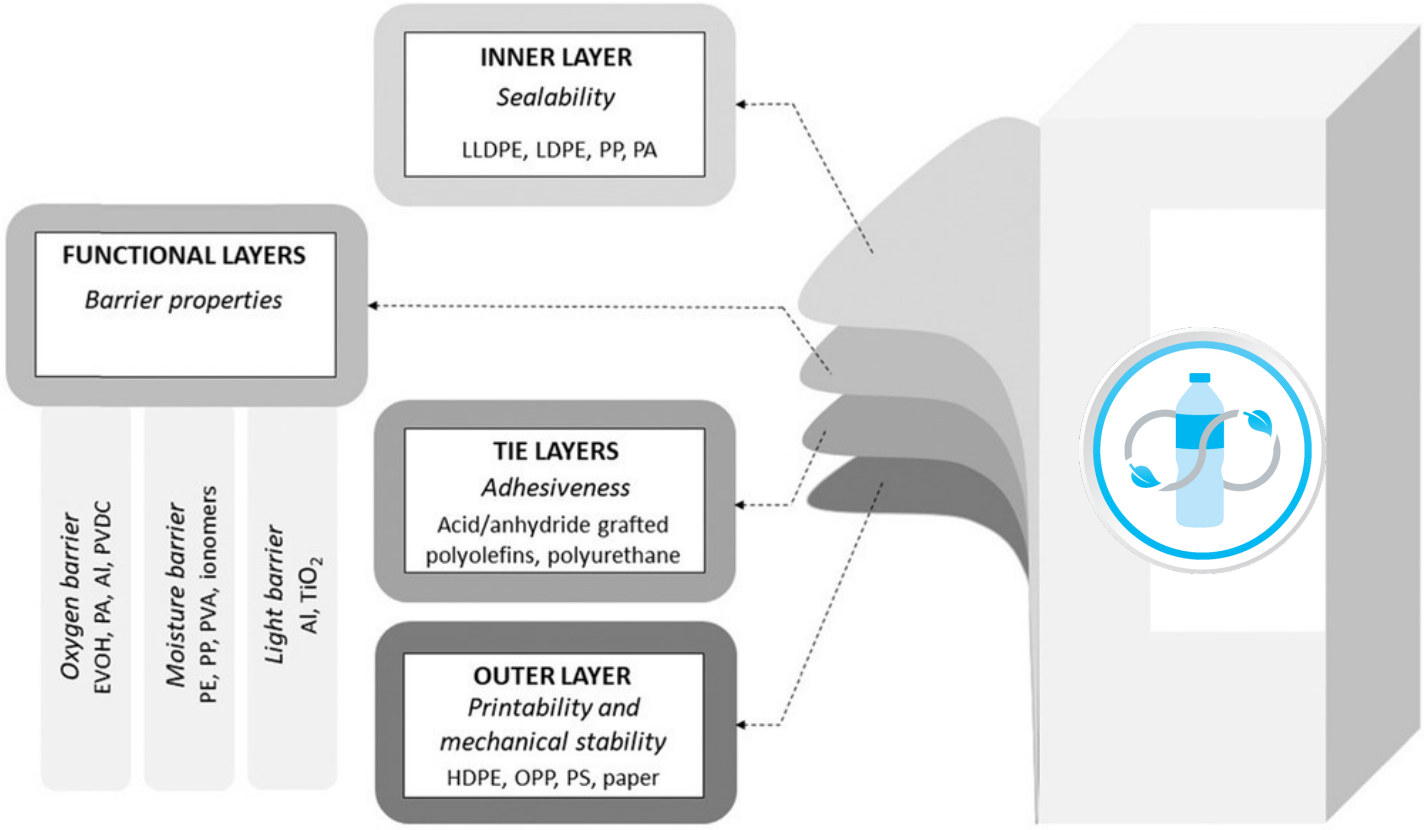
Overall goals:
- Develop sustainable packaging solutions for food products

Team size:
- 5 BOTTLE researchers

BOTTLE participants:
- CSU, NREL

BOTTLE tasks:
- Redesign, Modeling

BETO investment leveraged:
- Recyclable-by-design polymer portfolio[1]
- Poly(ID) and predictive modeling[2]



Multi-layer food packaging is not currently recyclable

[1]Shi *et al*. *Sci. Adv*. 2020; [2]Shi *et al*. *Chem* 2021

Patagonia/BOTTLE projects – Circularity for textiles

Chemical recycling of mixed textiles

~63% Plastics
~26% Cotton
~11% Other[1]

Dye removal, recovery, and recycling

[1]Morlet *et al*. *Ellen MacArthur Foundation Report: A New Textiles Economy* 2018; [2]Image: Scott, A. *C&EN* 2022

Patagonia – Project 1: Mixed textiles deconstruction

Overall goals:
- Develop a catalytic deconstruction technology to upcycle mixed plastic waste

Team size:
- 4 BOTTLE researchers

BOTTLE participants:
- NREL

BOTTLE tasks:
- Deconstruction, Characterization

BETO investment leveraged:
- Applied foundational knowledge in autoxidation developed via AOP funds to apply technology to mixed textiles[1]

[1]Sullivan, Werner, Ramirez, Ellis *et al*. *Science* 2022

Patagonia – Project 2: Textile pretreatments for recycling

Overall goals:

- Develop a biobased extraction process to remove dyes and additives from PET rich textiles to enable textile-to-textile recycling with integrated downstream separations to recover dyes

Team size:

- 5 BOTTLE researchers

BOTTLE participants:

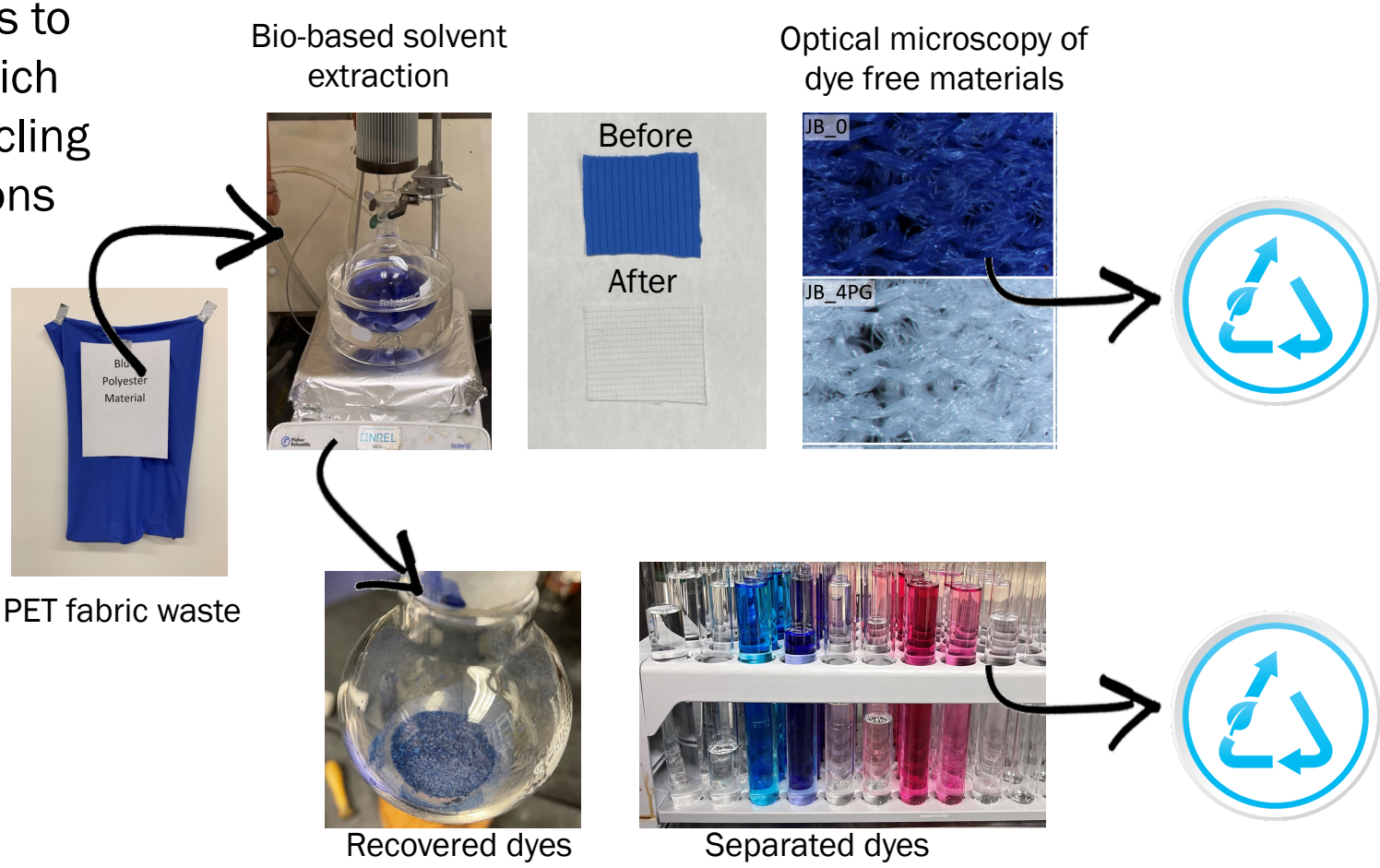
- NREL

BOTTLE tasks:

- Upcycling

BETO investment leveraged:

- Bio-based solvents from biomass[1]



[1]Stone, Webber *et al*. *Joule* 2022

P&G – Upcycling of polyethylene waste

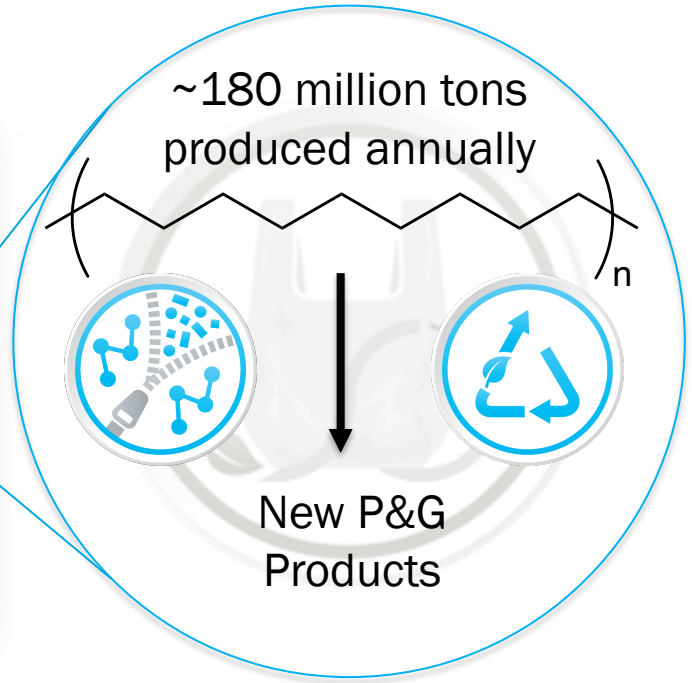
Overall goals:
- Develop a catalytic deconstruction technology to upcycle polyethylene waste

Team size:
- 5 BOTTLE researchers

BOTTLE participants:
- MIT, NREL

BOTTLE tasks:
- Deconstruction, Upcycling

BETO investment leveraged:
- Applying foundational knowledge in oxidation catalysis and deconstruction of polythylene[1,2]



[1]Sullivan, Werner, Ramirez *et al. Science* 2022; [2]Ellis, Rorrer, Sullivan *et al. Nature Catalysis* 2021.

– Deconstruction & upcycling of chlorinated plastics

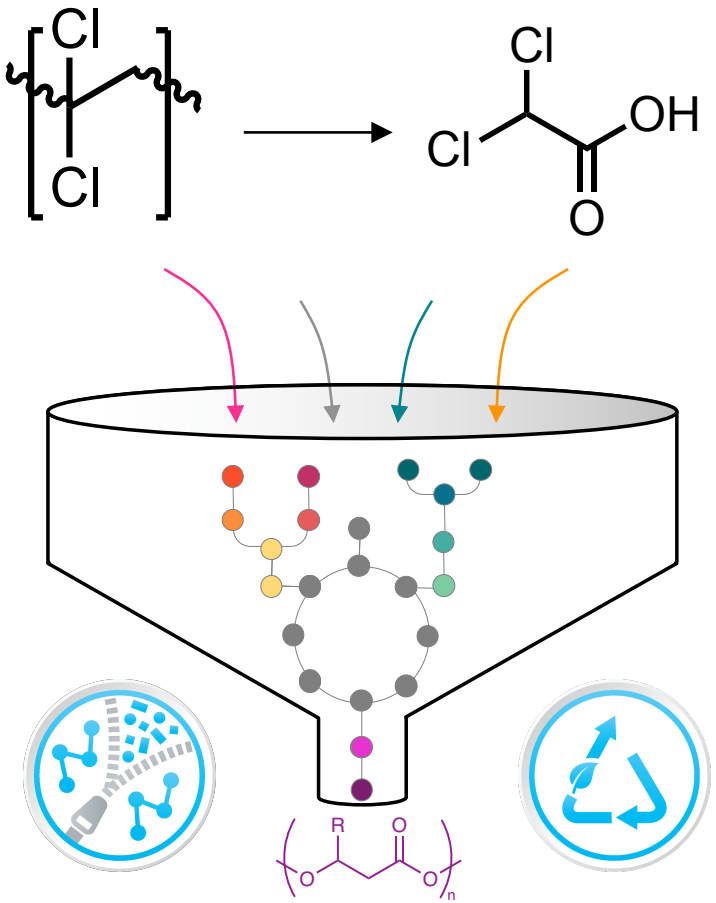
Overall goals:
- Develop an oxidative biological funneling technology to upcycle PVDC/PVC waste

Team size:
- 5 BOTTLE researchers

BOTTLE participants:
- NREL

BOTTLE tasks:
- Deconstruction, Upcycling

BETO investment leveraged:
- Applied foundational knowledge in oxidation catalysis and *P. putida* engineering[1,2]



[1]Werner *et al. Met. Eng.* 2021; [2]Sullivan, Werner, Ramirez *et al. Science* 2022

– Upcycling of HIPs electronic waste

CANON VIRGINIA, INC.

Overall goals:

- Develop a green pretreatment technology for high impact polystyrene (HIPs) to yield a high-quality product for e-waste recycling

Team size:

- 5 BOTTLE researchers

BOTTLE participants:

- MIT, NREL

BOTTLE tasks:

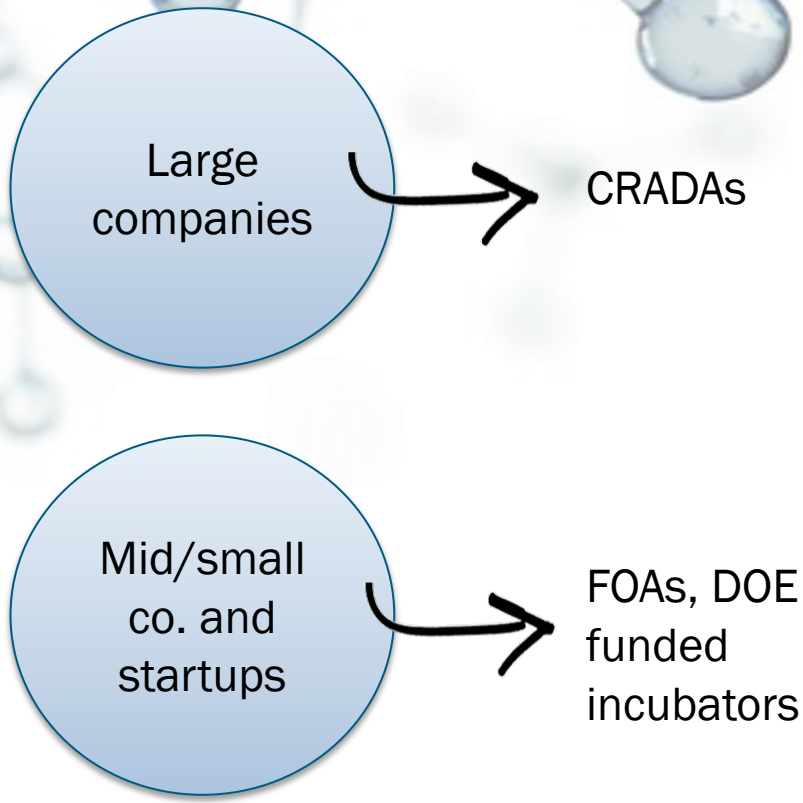
- Upcycling

BETO investment leveraged:

- Applied foundational knowledge in green chemistry and bio-based solvents

Impact

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



Quad Chart

Timeline

- Active Project Duration: 10/1/2020 – 9/30/2023
- Total Project Duration: 10/1/2019 – 9/30/2023

	FY23 Funding	Total Award (FY21-23)
DOE Funding	$10,000,000	$30,000,000

Project Partners

ANL, CSU, LANL, MIT, MSU, NREL, NU, ORNL, SLAC, UoP

TRL at Project Start: 1
TRL at Project End: 4

Funding Mechanism

Bioenergy Technologies Office FY21 AOP Lab Call (DE-LC-000L079) – 2020

Project Goals

- 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
- Work with industry to catalyze new upcycling paradigms and novel feedstocks

End of Project Milestones

- Deconstruction: Achieve hydrogenolysis of polyolefins in a continuous process with a selectivity profile of >60% to a single product. Deliver cutinase variants with the ability to reach over 80% conversion extent on crystalline PET in a pH-controlled bioreactor.
- Upcycling: Deliver a submission-ready manuscript that describes consolidated bioprocessing of PET plastic to an RBD monomer using a thermophilic microorganism.
- Redesign: Deliver a submission-ready manuscript on designer PHB with PE/PP-like performance via controlling stereomicrostructures that includes TEA, LCA, and biodegradation studies.
- Analysis: Deliver designs on autoxidation, hydrogenolysis, PET conversions, and at least 5 redesigned polymers in accordance with the primary BOTTLE metrics of carbon, economics, energy, and GHG emissions
- Modeling: Deliver an integrated set of tools that enable prediction of RBD polymers for a target application and their syntheses

Thank you!

Argonne NATIONAL LABORATORY

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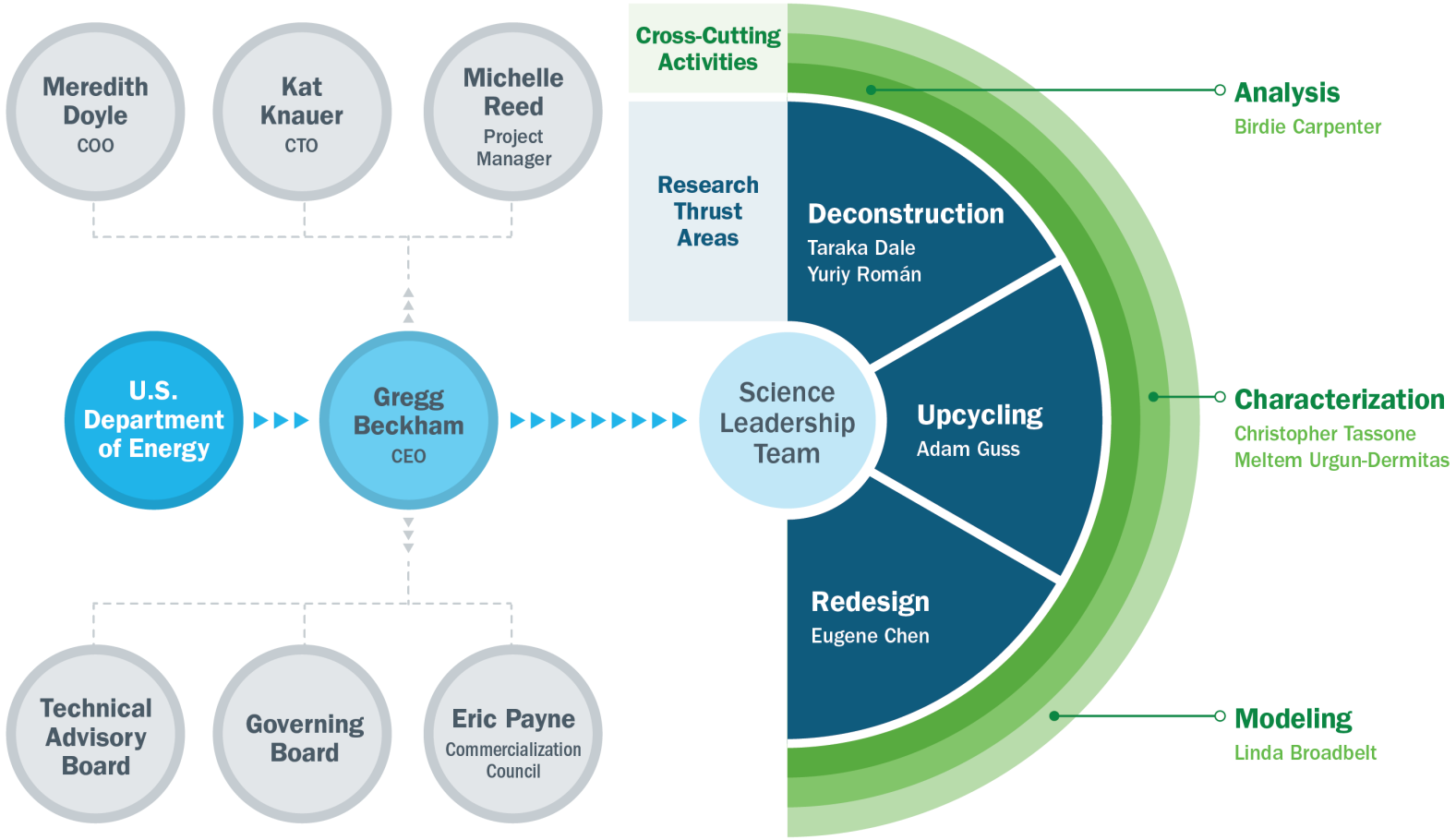
Rory Miles
Joy Watts
Luisana Avilan
Paul Cox
Raj Gill
Gerhard Konig
Bruce Lichtenstein
Michael Zahn

Additional Slides

Leadership Team Structure



BOTTLE Leadership Team (LT):

- CEO, COO, & PM
- Oversee the Management task
- *Role focused on leadership of BOTTLE*

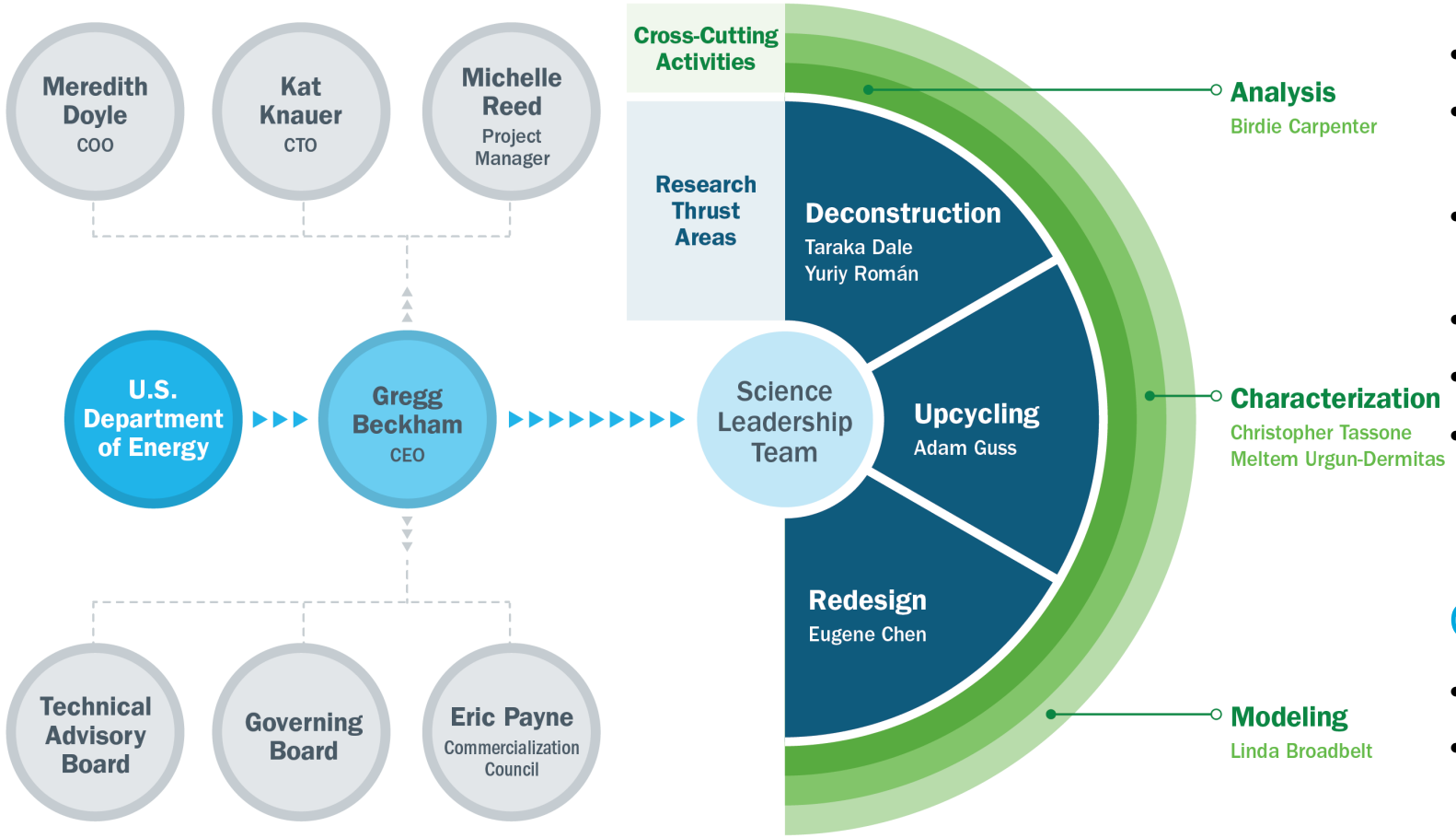
Governing Board (GB):

- BOTTLE LT, lab and several univ. leads, DOE
- Yearly strategic planning meeting
- *Role focused on management, strategy*

Science Leadership Team (SLT):

- CEO, all institutional leads, DOE
- Yearly planning meeting, teleconferences quarterly
- *Role focused on research execution*
- Annual Portfolio Review responsibilities
- Implement and supervise research projects at each institution

Technical Advisory Board and Comm. Council



Technical Advisory Board (TAB):

- Feedback on R&D, operations, management
- Invited diverse group of thought leaders from academia, government, industry, non-profits
- TAB represents key points in the plastics value chain to ensure robust assessment of BOTTLE
- Convene annually with the All-hands meeting
- Provide written evaluations to DOE, BOTTLE LT
- Includes leads of complementary R&D efforts in this space

Commercialization Council:

- Representative from each partner institution
- Central “storefront” for accessing BOTTLE IP through partnership and licensing
- Promote rapid deployment of BOTTLE IP

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.

In revision

Anelia Milbrandt, Kamyria Coney, Alex Baggett, Gregg T. Beckham, Quantity, distribution, market value, and energy value of plastic waste in the United States, in revision at Resources, Conservation, and Recycling.

Allison Z. Werner, Rita Clare, Thomas D. Mand, et. al, Tandem chemical deconstruction and biological upcycling of poly(ethylene terephthalate) to b-ketoadipic acid by Pseudomonas putida KT2440, In revision at Metabolic Engineering.

In press

Scott R. Nicholson, Julie E. Rorrer, Avantika Singh, Mikhail O. Konev, Nicholas A. Rorrer, Alberta C. Carpenter, Alan J. Jacobsen, Yuriy Román-Leshkov, Gregg T. Beckham, The critical role of process analysis in chemical recycling and upcycling of waste plastics, in press at Ann. Rev. Chem. Biomolec. Eng.

Publications

2023

Taylor Uekert, Avantika Singh, Jason S. DesVeaux, Tapajyoti Ghosh, Arpit Bhatt, Geetanjali Yadav, Shaik Afzal, Julien Walzberg, Katrina M. Knauer, Scott R. Nicholson, Gregg T. Beckham, and Alberta C. Carpenter, "Technical, economic, and environmental comparison of closed-loop recycling technologies for common plastics," ACS Sustainable Chemistry & Engineering (2023) 11, 3, 965–978.

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Kevin P. Sullivan, Allison Z. Werner, Kelsey J. Ramirez, et. al., Mixed plastics waste valorization through tandem chemical oxidation and biological funneling, Science (2022) 378, 207-211.

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Publications

Julie E. Rorrer, Amani M. Ebrahim, Ydna Questell-Santiago, Jie Zhu, Clara Troyano-Valls, Arun S. Asundi, Anna E. Brenner, Simon R. Bare, Christopher J. Tassone, Gregg T. Beckham, and Yuriy Román-Leshkov, The role of bifunctional Ru/acid catalysts in selective hydrocracking of polyethylene and polypropylene waste to liquid hydrocarbons, *ACS Catal*. (2022) 12, 22, 13969–13979.

Andrea H. Westlie, Eugene Y.-X. Chen, Chris M. Holland, Shannon S. Stahl, Meredith Doyle, Scott R. Trenor, Katrina M. Knauer, Polyolefin innovations towards circularity and sustainable alternatives, *Macromolecular Rapid Communications* (2022) 43, 2200492.

Raka G. Dastidar, Min Soo Kim, Panzheng Zhou, Zaneta Luo, Changxia Shi, Kevin J. Barnett, Daniel J. McClelland, Eugene Y.-X. Chen, Reid C. Van Lehn, George W. Huber, Catalytic production of tetrahydropyran (THP): a biomass-derived, economically competitive solvent with demonstrated use in plastic dissolution, *Green Chem*. (2022) 24, 9101–9113.

Zhen Zhang, Changxia Shi, Miriam Scoti, Xiaoyan Tang, and Eugene Y.-X. Chen, Alternating Isotactic Polyhydroxyalkanoates via Site- and Stereoselective Polymerization of Unsymmetrical Diolides, *J. Am. Chem. Soc. (*2022), 144, 20016–20024.

Andrea H. Westlie, Ethan C. Quinn, Celine R. Parker, Eugene Y.-X. Chen, Synthetic biodegradable polyhydroxyalkanoates (PHAs): recent advances and future challenges, *Prog. Polym. Sci.* (2022), 134, 101608.

Erika Erickson, Japheth E. Gado, Luisana Avilán, et al., Sourcing thermotolerant poly(ethylene terephthalate) hydrolase scaffolds from natural diversity, *Nat Comm. (*2022) 13, 7850.

Robin M. Cywar, Nicholas A. Rorrer, Heather B. Mayes, Anjani K. Maurya, Christopher J. Tassone, Gregg T. Beckham, Eugene Y.-X. Chen, Redesigned hybrid nylons with optical clarity and chemical recyclability, *J. Am. Chem. Soc.* (2022) 144, 5366–5376.

Publications

Coralie Jehanno, Jill W. Alty, Martijin, Steven De Meester, Andrew P. Dove, Eugene Y.-X Chen, Frank A. Leibfarth, Haritz Sardon, Critical advances and future opportunities in upcycling commodity polymers, *Nature* (2022), 603, 803–814.

William M. Kincannon, Michael Zahn, Rita Clare, Jessica Lusty Beech, Ari Romberg, James Larson, Brian Bothner, Gregg T. Beckham, John E. McGeehan, and Jennifer L. DuBois, Biochemical and structural characterization of an aromatic ring-hydroxylating dioxygenase for terephthalic acid catabolism. *Proc. Natl. Acad. Sci. (*2022) 19(13):e2121426119.

Jessica Lusty-Beech, Rita Clare, William M. Kincannon, Erika Erickson, John E. McGeehan, Gregg T. Beckham, Jennifer L. DuBois, A flexible kinetic assay efficiently sorts prospective biocatalysts for PET plastic subunit hydrolysis. *RSC Adv.* (2022) 12, 8119-8130.

Changxia Shi, Ryan W. Clarke, Michael L. McGraw, Eugene Y.-X., Closing 'one monomer–two polymers–one monomer' loop via orthogonal (de)polymerization of a lactone/olefin hybrid, J*. Am. Chem. Soc.* (2022) 144, 2264−2275.

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Presentations

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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

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

Presentations

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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

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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

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