# **Plastics Innovation Challenge Draft Roadmap**

U.S. Department of Energy





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# List of Acronyms

AMO	Advanced Manufacturing Office
ARPA-E	Advanced Research Projects Agency-Energy
BER	Biological and Environmental Research
BES	Basic Energy Sciences
BETO	Bioenergy Technologies Office
BOTTLE	Bio-Optimized Technologies to keep Thermoplastics out of Landfills and the Environment
DOE	U.S. Department of Energy
FOA	funding opportunity announcement
GHG	greenhouse gas
PET	polyethylene terephthalate
PIC	Plastics Innovation Challenge
R&D	research and development
REMADE	Reducing EMbodied-energy And Decreasing Emissions

# **Executive Summary**

Plastics have evolved tremendously and now serve many purposes in modern life, delivering a broad range of benefits. Plastics are versatile, durable, and lightweight and are cost-effective compared to many other materials, making them desirable in many applications. They are critical to the safe and economical distribution of food globally, make up energy-efficient packaging, provide lightweighting options to reduce the energy consumed by cars and airplanes, and are key components of many medical devices and safety equipment. Annually, over 300 million metric tons of new plastic are generated globally and only a small percentage is recycled. Most plastic waste ends up in landfills, but plastics also leak into the environment, representing an environmental challenge.

Of particular importance to the U.S. Department of Energy (DOE) is the opportunity to improve the energy efficiency, environmental performance, and process efficiency of energy-intensive and waste-intensive industries.<sup>1</sup> Also of importance are opportunities for new bioproducts.<sup>2</sup> Approximately 2% of total energy consumption in the United States is used to manufacture plastics, resins, and synthetic rubber.<sup>3</sup> Plastic production also uses nearly 6% of global oil production, representing a large opportunity for further energy and process efficiency improvements.<sup>4</sup> The Plastics Innovation Challenge (PIC) was launched in 2019 to make domestic processing of plastic waste more economically viable and energy-efficient, develop new and improved plastic materials lacking the end-of-life concerns as incumbent materials, and ultimately reduce plastic waste accumulation.

Four strategic goals focus the scope of the Plastics Innovation Challenge:

- 1. <u>Deconstruction</u>: Create new chemical, thermal, and biological pathways to deconstruct plastics efficiently into useful chemical intermediates
- 2. <u>Upcycling</u>: Advance the scientific and technological foundations that will underpin new technologies for upcycling chemical intermediates from plastic waste into higher-value products
- 3. <u>Recyclable by Design</u>: 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. <u>Scale and Deploy</u>: 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.

This roadmap outlines the challenges and opportunities facing PIC efforts, and these areas of opportunity frame PIC research directions. A lack of robust chemical and biological mechanisms limits the deconstruction of existing plastics (Goal 1). This is further complicated by the need for more robust processes that can convert diverse and contaminated plastic waste streams into useful chemical intermediates that can be upcycled into higher-value products (Goals 1 and 2). Finally, even when robust processes are developed to deconstruct existing plastics, the demand for plastics remains, leading to a critical need for new plastic materials that have the same advantages as current plastics but can be economically recycled or biodegraded safely in the environment (Goals 1, 2, 3, and 4). To have an impact, new technology pathways must scale in an economically competitive way (Goal 4).

This roadmap identifies key research needs and opportunities for DOE-sponsored research and development and catalogs challenges and opportunities facing PIC efforts. With a concerted and coordinated research and development effort, the U.S. Department of Energy's Plastics Innovation Challenge aims to transform our approach to plastic waste and develop new classes of plastic that are recyclable and upgradeable by design.

<sup>&</sup>lt;sup>1</sup> Energy Efficiency, U.S. Code 42 (2007), § 16191(a)(2)(C).

<sup>&</sup>lt;sup>2</sup> Bioenergy Program, U.S. Code 42 (2007), § 16232(b).

<sup>&</sup>lt;sup>3</sup> U.S. Energy Information Administration. 2017. "2014 Manufacturing Energy Consumption Survey."

<sup>&</sup>lt;sup>4</sup> Ellen MacArthur Foundation. 2017. *The New Plastics Economy: Rethinking the Future of Plastics & Catalysing Action*. Cowes, United Kingdom: Ellen MacArthur Foundation.

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# Introduction

# **Overview of Plastic Production and Waste Generation**

Plastics are a synthetic material made from organic polymers, including derivatives of polyethylene, polypropylene, polystyrene, polyurethanes, polyamides, and polyesters. Plastics have become an integral part of modern life and provide tremendous benefits—from safer food to lighter, more fuel-efficient vehicles.

Proliferation of plastic production and waste (Figure 1) poses a growing environmental crisis. Each year, the global economy produces over 380 million metric tons (Mt) of new plastic material and generates over 280 Mt of plastic waste from end-of-life plastic products, with 40% of the waste deposited into landfills and nearly 20% dispersed into the environment.<sup>5</sup> Recycling plastics may reduce energy costs by more than 50% compared to virgin plastic production.<sup>6</sup> Unfortunately, the vast majority of plastics are never recycled.



Figure 1. Total global 2015 production and waste generation of the most common commodity polymers

(HDPE: high-density polyethylene; LDPE: low-density polyethylene; LLDPE: linear low-density polyethylene; PET: polyethylene terephthalate; PP: polypropylene; PP&A: polyester, polyamide, and acrylic; PS: polystyrene; PUR: polyurethane; PVC: polyvinylchloride)<sup>7</sup>

Current recycling strategies often do not allow for cost-effective recycling of commonly used plastics. The magnitude of the problem is vast:

• Approximately 80% of plastic waste has accumulated in landfills and the natural environment<sup>8</sup>

<sup>&</sup>lt;sup>5</sup> Ellen MacArthur Foundation. *The New Plastics Economy*.

<sup>&</sup>lt;sup>6</sup> Nicholas A. Rorrer, Scott Nicholson, Alberta Carpenter, Mary J. Biddy, Nicholas J. Grundl, and Gregg T. Beckham. 2019. "Combining Reclaimed PET with Bio-based Monomers Enables Plastics Upcycling." *Joule* 3(4): 1006–1027. https://doi.org/10.1016/j.joule.2019.01.018.

<sup>&</sup>lt;sup>7</sup> Roland Geyer, Jenna R. Jambeck, and Kara Lavender Law. 2017. "Production, use, and fate of all plastics ever made." *Science Advances* 3(7): e1700782. https://doi.org/10.1126/sciadv.1700782.

<sup>&</sup>lt;sup>8</sup> Geyer, Jambeck, and Law. "Production."

• Only 14% of plastic packaging produced each year is collected for recycling and only 2% is recycled into the same or similar-quality products.<sup>9</sup>

Plastics recycling represents an energy efficiency opportunity:

- Approximately 2% of total energy consumption in the United States is used to manufacture plastics, resins, and synthetic rubber, emitting substantial greenhouse gas (GHG) emissions across the whole plastic life cycle.<sup>10</sup>
- Globally, plastics production totals 3.8% of annual GHG emissions.<sup>9,11,12</sup> Resin generation produces the bulk of GHG emissions associated with conventional plastics, contributing 61% of the GHG emissions attributed to plastic production.<sup>13</sup>
- Six percent of the world's petroleum is used to make plastic, and plastics that end up in landfills represent a potential energy opportunity.<sup>9</sup>
- Ninety-eight percent of plastic packaging is made from virgin feedstock.9

The plastic waste problem continues to grow in importance in terms of energy. Plastic production is projected to continue to increase substantially through 2050 (Figure 2), even as oil and natural gas production is projected to shrink under a high renewable penetration scenario (Figure 3). This would lead to a situation in which plastics may account for up to 20% of global petrochemical consumption by 2050, increasing the demand on non-renewable feedstocks for plastics production.



Figure 2. Realized and predicted production of commodity plastics through 205014,15

<sup>&</sup>lt;sup>9</sup> Ellen MacArthur Foundation. The New Plastics Economy.

<sup>&</sup>lt;sup>10</sup> U.S. Energy Information Administration. 2017. "2014 Manufacturing Energy Consumption Survey." Washington, D.C.: EIA. Table 1.2.

<sup>&</sup>lt;sup>11</sup> Center for International Environmental Law. 2019. Plastic & Climate: The Hidden Costs of a Plastic Planet. Washington, D.C.: Center for International Environmental Law.

<sup>&</sup>lt;sup>12</sup> Jiajia Zheng and Sangwon Suh. 2019. "Strategies to reduce the global carbon footprint of plastics." *Nature Climate Change* 9: 374–378. https://doi.org/10.1038/s41558-019-0459-z.

<sup>&</sup>lt;sup>13</sup> Zheng and Suh. "Strategies."

<sup>&</sup>lt;sup>14</sup> International Renewable Energy Agency (IRENA). 2018. Global Energy Transformation: A Roadmap to 2015. Abu Dhabi: IRENA.

<sup>&</sup>lt;sup>15</sup> International Energy Agency (IEA). 2018. The Future of Petrochemicals. Paris: IEA.



Figure 3. Predicted oil and gas demand through 2050 for a business-as-usual scenario (dots) and high renewable penetration scenario (dashes)<sup>16,17</sup>

# **Limits of Current Recycling**

Recycling, collection, and sorting strategies are often inefficient, leading to long transportation distances that ultimately end up disposing contaminated products as waste and leaking plastics into the environment. Standard municipal recycling facilities may take in acceptable, recyclable mixed-plastic waste and mechanically break it down into pellets that are then reformed into new materials through melt extrusion and molding. In this process, the quality of the processed material is reduced, limiting the value of and uses for the recycled product. Substantial room for technological improvement exists here. Namely, the quality of the starting plastic waste can be maintained by selective chemical or biological decomposition followed by upgrading into a new material. The current recycling process is also limited because it cannot accept multilayer packaging or thin-film packaging, which comprise 8% of all plastics produced annually.

In response to traditional recycling limitations, research and development (R&D) efforts have enabled commercialization of biodegradable thermoplastic materials from biologically derived polylactic acid and from biopolymers such as polyhydroxybutyrates (PHBs) and polyhydroxyalkanoates (PHAs). Despite the advantage of biodegradability, the material properties are not suitable for many applications due to the low flexibility of current-generation bioplastics and limited number of suitable applications. New materials with improved recyclability or biodegradability—and equivalent functionality—have the potential to vastly reduce plastic waste accumulation and improve recovery and reuse of an energy-rich feedstock. However, knowledge gaps limit the design and development of these new and improved plastic materials.

### **DOE** and the Plastics Innovation Challenge

Recognizing the need for plastic recycling solutions, the U.S. Department of Energy (DOE) launched the Plastics Innovation Challenge (PIC) in November 2019. The PIC seeks to dramatically reduce plastic waste and position the United States as the world leader in advanced plastic recycling and upcycling technologies, enabling American companies to develop and deploy innovative technologies. DOE is especially suited to

<sup>&</sup>lt;sup>16</sup> IRENA. Global Energy Transformation.

<sup>&</sup>lt;sup>17</sup> IEA. Future of Petrochemicals.

tackle the plastics challenge, possessing capabilities in critical science and technology areas needed to address energy recovery and energy savings in plastic production while reducing plastic waste. New technologies that may help recycle current plastic waste will recover the energy-rich carbon building blocks that would otherwise be lost. Similarly, DOE is suited to invest in science and technologies to create new materials designed with the material life cycle in mind, including the expertise to generate the material and develop the technologies to facilitate energy and carbon recovery at the material's end of life.

To meet the PIC goals, DOE will leverage decades of research in key areas such as biopolymer deconstruction, catalysis science, genomic science, materials science, techno-economic and life cycle analysis, and biosystems design. Further, DOE has fostered a strong scientific infrastructure network within the National Laboratory system, including scientific user facilities. DOE has state-of-the-art facilities and leading experts poised to develop innovative solutions to tackle the PIC.

### **Roadmap Goals**

This roadmap serves to:

- Communicate the goals, impact, challenges, and research directions of the Plastics Innovation Challenge
- Enable coordination of research efforts across DOE and with other federal agencies
- Engage stakeholders to develop common goals across the entire breadth of organizations, science, and technology spanned by the PIC research and development effort
- Describe a path for transforming current discarded plastics from a waste to a resource for making new, high-value products.

# 2030 Vision, Mission, and Strategic Goals

The PIC spans the full research, development, and deployment spectrum to address key challenges that limit plastic recycling. Fundamental research investments will cover the discovery of novel approaches for plastic synthesis and deconstruction.

A concerted effort across fundamental and applied levels of investigation will be required within the framework of the PIC.

The vision, mission, and strategic goals of the PIC are designed to position the United States as a leader in science and technology innovations needed to develop and manufacture new plastic technologies.

#### Vision

The United States leads the world in developing and deploying technologies that minimize plastic waste and promote energy-efficient and economic plastic and bioplastic design, production, reuse, and recycling.

#### **Mission**

PIC's mission is to deliver transformative science and technology solutions that will reduce plastic waste and lower the energy impacts of plastic production and reuse.

### **Strategic Goals**

- 1. Develop biological, chemical, and thermal methods for **deconstructing** plastic wastes into useful chemicals
- 2. Develop technologies to **upcycle** waste chemical streams into higher-value products, encouraging increased recycling

- 3. 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. 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.

#### **Objectives/Metrics**

- Develop technologies to address end-of-life fate for >90% of plastic materials<sup>a</sup>
- Provide ≥50% energy savings relative to virgin material production<sup>b</sup>
- Achieve  $\geq$ 75% carbon utilization from waste plastics to encourage material-efficient processes<sup>c</sup>
- Develop recyclable-by-design plastic solutions that are **cost-competitive** with incumbent plastic materials and processes.<sup>d</sup>

<sup>a</sup> Of the 285 Mt of plastic waste generated globally in 2015, 91% by mass was from just five classes of polymers: polyolefins (low-density polyethylene, linear low-density polyethylene, high-density polyethylene, and polypropylene), polystyrenes, polyesters, polyamides, and polyurethanes. By targeting solutions for these classes of materials, the PIC can create effective recycling technologies for the large majority of modern plastic waste.<sup>18</sup>

- <sup>b</sup> Fifty percent energy savings relative to virgin material production has been achieved using chemical and mechanical recycling techniques and defines a reasonable baseline target for newly developed processes.<sup>19</sup>
- <sup>c</sup> PET bottles are among the most efficiently recycled plastic products. Even so, current mechanical recycling processes in the United States are able to convert on average only ~66.6% of the collected bottles into clean flake, while the remainder is landfilled. The PIC seeks to improve recycling and upcycling technologies for PET as well as other major polymer classes to exceed 75% carbon retention, which will show improvement in carbon recycling efficiency for PET as well as other major polymer classes.<sup>20</sup>
- <sup>d</sup> Cost-competitiveness with incumbent materials will be calculated on a per-application basis, as some redesigned plastics may use more or less material to achieve a similar function.

# **Challenges and Opportunities**

Challenges help identify where DOE efforts can help achieve the long-term vision of the PIC. Prior analysis and coordination efforts within DOE and with external partners have identified key opportunities and challenges facing plastic waste mitigation. Plastic waste mitigation includes the direct reduction of existing plastic waste and the introduction of new recyclable-by-design or biodegradable plastic materials designed to displace today's non-recyclable plastics. These opportunities and challenges were drawn from the following DOE and stakeholder reports:

<sup>&</sup>lt;sup>18</sup> Geyer, Jambeck, and Law. "Production."

<sup>&</sup>lt;sup>19</sup> AliReza Rahimi and Jeanette M. Garcia. 2017. "Chemical recycling of waste plastics for new materials production." *Nature Reviews Chemistry* 1: 0046. https://doi.org/10.1038/s41570-017-0046.

<sup>&</sup>lt;sup>20</sup> National Association for PET Container Resources (NAPCOR). 2018. *Postconsumer PET Container Recycling Activity in 2017*. Charlotte, NC: NAPCOR. https://napcor.com/wp-content/uploads/2018/11/NAPCOR\_2017RateReport\_FINAL.pdf.

The Bioenergy Technologies Office (BETO) and Advanced Manufacturing Office (AMO) hosted the "Plastics for a Circular Economy Workshop." Stakeholders from industry, National Laboratories, academia, and government agencies contributed to the conclusions in the workshop report.<sup>21</sup>

The Reducing EMbodied-energy And Decreasing Emissions (REMADE) Institute hosted a workshop on "Remanufacturing, Repair, and Reuse" and published a technology roadmap.<sup>22</sup>

DOE's Office of Science Basic Energy Sciences (BES) program hosted a "Roundtable on Chemical Upcycling of Polymers" to identify the fundamental challenges and research opportunities that could accelerate the transformation of discarded plastics to higher-value fuels, chemicals, and materials.<sup>23</sup>

The Biological and Environmental Research (BER) program hosted a workshop on "Genome Engineering for Material Synthesis" to explore opportunities and challenges for leveraging synthetic biology and computational tools in the synthesis of novel biomaterials.<sup>24</sup>







<sup>&</sup>lt;sup>21</sup> U.S. Department of Energy Office of Energy Efficiency and Renewable Energy (EERE). 2020. *Plastics for a Circular Economy Workshop: Summary Report*. Washington, D.C.: EERE. DOE/EE-2074. https://www.energy.gov/eere/bioenergy/downloads/plastics-circular-economy-workshop-summary-report.

report. <sup>22</sup> REMADE Institute. 2019. *REMADE Institute Technology Roadmap 2019*. West Henrietta, NY: REMADE Institute. https://remadeinstitute.org/technology-roadmap.

<sup>&</sup>lt;sup>23</sup> U.S. Department of Energy. 2019. *Roundtable on Chemical Upcycling of Polymers*. Washington, D.C.: DOE. https://science.osti.gov/-/media/bes/pdf/BESat40/Polymer\_Upcycling\_Brochure.pdf.

<sup>&</sup>lt;sup>24</sup> U.S. Department of Energy. 2019. *Genome Engineering for Materials Synthesis: Workshop Report*. Washington, D.C.: DOE. DOE/SC-0198. https://genomicscience.energy.gov/biosystemsdesign/gems/index.shtml.

The National Academy of Sciences, with DOE involvement, held a workshop "Closing the Loop on the Plastics Dilemma."<sup>25</sup>

The Office of Fossil Energy's Office of Clean Coal and Carbon Management published their strategic vision, highlighting future efforts on co-firing plastics, CO<sub>2</sub> conversion to plastics, and manufacturing of plastics from coal and byproducts, and released a Hydrogen Strategy highlighting the need to address several key challenges, including gasification of plastics.<sup>26</sup>





The PIC addresses the whole plastic life cycle, from recovering existing plastic waste and enabling upcycling technologies to the development of next-generation plastic materials. The PIC will work to reach their 2030 vision by focusing on the challenges facing each of the strategic goals: deconstruction, upcycling, recyclable-by-design materials, and scaling/deploying. Based on feedback received from experts and stakeholders through the aforementioned avenues, the following R&D needs were identified.

# **Challenges Facing the PIC Strategic Goals**

#### Deconstruction

Deconstruction efforts are needed to develop new chemical and biological pathways to efficiently break down plastics into useful chemical intermediates that can be recycled to the starting material or upcycled into more valuable products. Scientific advances in chemistry, synthetic biology, computational science, and data science will be critical to discovering new approaches for energy- and atom-efficient deconstruction and conversion of plastics to high-value products. Some broad challenges include:

- Development of selective methods for specific plastics, as well as broad methods to process mixed and contaminated waste streams
- Development of deconstruction approaches for flexible plastic packaging, including multilayer materials, which are not currently recyclable
- Integration and scaling of innovations to facilitate industry adoption and commercialization.

<sup>&</sup>lt;sup>25</sup> National Academy of Sciences, Engineering, and Medicine. 2020. *Closing the Loop on the Plastics Dilemma: Proceedings of a Workshop-in Brief.* Washington, D.C.: The National Academies Press. https://doi.org/10.17226/25647.

<sup>&</sup>lt;sup>26</sup> U.S. Department of Energy. 2020. Office of Clean Coal and Carbon Management: Strategic Vision 2020–2024. Washington, D.C.: DOE. https://www.energy.gov/sites/prod/files/2020/08/f77/FE-20%20Strategic%20Vision%20FINAL%202020\_Aug\_12\_compliant.pdf.

#### Chemical Deconstruction

Polymers—the molecules that make up plastics—are long organic chains with stable chemical bonds that typically require high-temperature deconstruction processes to yield a mixture of smaller intermediates. Chemical deconstruction includes both selective and nonselective methods, each of which faces unique challenges.

- Selective deconstruction methods provide an opportunity for efficient and controlled depolymerization of plastic waste into a known intermediate that can be effectively recycled.
  - Selective catalytic depolymerization, solvent-based methods, and reactive depolymerization all show promise as nascent deconstruction technologies but are susceptible to feedstock variability and contamination.
- Nonselective thermal deconstruction methods such as gasification and pyrolysis may be able to accept mixed feedstocks and may be more resilient to contamination.
  - The development of advanced catalysts, syngas cleaning technologies, oxygen separation, and H<sub>2</sub>/CO<sub>2</sub> separation processes are necessary to address contaminant issues and reduce capital costs of these nonselective deconstruction approaches.
- Deconstruction approaches are necessary to enable recycling of multilayer packaging.
  - Deconstruction of multilayer packaging depends on improvements in mechanical preprocessing, material separations, delamination, and chemical methods to deconstruct the multicomponent structure.

#### **Biological Deconstruction**

Similar to chemical deconstruction, selective and nonselective biological deconstruction approaches exist but face their own unique challenges.

- Selective approaches include targeted degradation using specific enzymatic pathways, either *ex situ* or *in vivo*.
  - New plastic-degrading enzymes still need to be discovered, particularly those that can function at elevated temperatures.
  - Engineering new enzymes or organisms to degrade plastic represents a major challenge. Enzyme structure does not always predict function, and organism metabolism has only coevolved with plastic materials for a short period of time.
- Nonselective processes include biodegradation of plastic through complex microbial metabolic pathways, ultimately converting the material to microbial cell mass and CO<sub>2</sub>. Several synthetic polymers are already known to be targets of microbial enzymatic deconstruction, and additional relevant enzymes and pathways likely exist in nature.
  - Fundamental research is required to isolate and characterize novel enzymes and metabolic pathways for further development.
  - Complex microbiomes can be leveraged to degrade polymers, but gaining mechanistic understanding of the conversion of polymers, the breakdown of their products, and the synthesis of novel bioproducts remain significant challenges.

- Better standards for composting and biodegradability are needed to provide researchers access to extensive degradation studies under standardized conditions.
- Most polymers, including polypropylene and polyethylene, may be especially difficult to degrade biologically because they are not soluble in the aqueous solutions required for enzyme activity and microorganism survival.
- The heterogeneity of mixed-plastic waste streams poses a challenge to all biological deconstruction efforts because each plastic polymer class will require a unique metabolic pathway.

#### Upcycling

Upcycling efforts generate valuable products from discarded plastics. Development of new upcycling technologies requires the discovery of scalable and economically viable biological and chemical mechanisms for coupling deconstruction with reconstruction into new products or similar processes for functionalizing polymers and directly converting them into higher-value products. Compatibilization of polymers, without deconstruction, may also enable upcycling of mixed plastics into a more valuable composite material. In general, upcycling provides unique opportunities to rethink plastic design. The scope of these opportunities is enormous, and each opportunity faces its own set of limitations. Some challenges include:

- Integration of experimental, computational, and data science tools, particularly for real-time analysis, to elucidate the mechanisms and kinetics of deconstruction, reconstruction, and material performance of the upcycled product
- Understanding of the end-of-life impacts of the material on the environment, human health, and future recycling
- Discovery and understanding of markets for upgraded waste products to logically design upcycling processes.

#### Chemical Upcycling

Catalytic and synthetic approaches may be heavily leveraged in developing upcycling approaches and technologies. Improved catalysis can be employed to directly functionalize polymers and/or make desirable products such as chemicals, fuels, or new materials. Some challenges facing chemical upcycling include:

- Developing a detailed mechanistic understanding of chemical pathways and structure-function relationships to facilitate new material design
- Advancing new experimental and computational tools to probe and control chemical mechanisms for macromolecular transformations, including the use of machine-learning- or artificial-intelligence-based techniques and development of appropriate data sets.

#### **Biological Upcycling**

Biological diversity holds unique opportunities in relation to upcycling, because deconstruction and reconstruction can conceivably be coupled within the same organism. Some challenges facing biological upcycling include:

- Developing a molecular-, structural-, and systems-enabled understanding of microbial polymer deconstruction to enhance upcycling-related synthetic biology efforts
- Understanding how to constrain the large number of potential targets for the *de novo* design of metabolic solutions to upcycle polymers in the context of available microbial metabolic and synthetic biology capabilities
- Developing approaches to characterize biochemical mechanisms, leveraging complex metabolic interactions among enzymes and microbiomes, and bringing biological systems to scale.

#### **Recyclable by Design**

Recyclable-by-design plastics have the properties of today's plastics, are easily recycled, and can be manufactured at scale domestically. Recyclable-by-design plastics will maximize the economic value of waste plastics streams, incentivizing their closed-loop collection. Co-design of new polymeric materials with competitive properties and mechanisms for deconstruction and reconstruction is necessary to enable a circular plastics life cycle. In any of these cases, there is an opportunity to design the new material with the end of life in mind. Therefore, both product performance and the ability to reclaim value from the material at its end of life are essential. A key set of challenges facing the development of these materials includes:

- Understanding how polymer structure and chemical composition impart desired functionality and recyclability
- Incorporating labile chemical bonds must not decrease product performance
- Developing integrated approaches to the synthesis, breakdown, separation, upcycling, and manufacturing of the new plastics at scale, which must be considered holistically to enable a plastics circular economy
- Creating new technologies to convert alternative (non-petroleum) carbon feedstocks, especially CO<sub>2</sub>, to plastic monomers, enabling emerging end-of-life options such as advanced pyrolysis to complete a carbon-reducing circular life cycle
- Engineering microorganisms to produce polymers with characteristics similar or superior to incumbent petroleum-based plastics or further optimizing bio-based polymers with enhanced features for better end-of-life characteristics or recyclability for a more circular life cycle.

#### Scale and Deploy

Scale-and-deploy efforts support a domestic plastic upcycling supply chain. Scaling new technologies intrinsically includes improved collection, sorting, and mechanical recycling methods. Due to the amount of plastic manufacturing and the scope of the recycling need, scaling efforts face some significant challenges, including:

• Developing improved, optimized, and modern recycling technologies, including innovations in:

- Enhanced sorting technologies, which will allow for more immediate processing of complex mixed-waste streams
- Direct sorting of flexible plastic films/bags from rigid plastic products, which is an especially costly problem for municipal recycling facilities today
- Improved thermomechanical recycling that mitigates mechanical property degradation and will increase the business case for recycling plastics into the same materials (same-cycling)
- Compatibilizer innovation, such as specialty block polymers that improve the properties of comingled polymers, which will allow for processing of mixed-waste streams into a single, high-value mixed resin.
- Creating frameworks for assessing energy and environmental impacts of plastics from cradle to grave, which support a comprehensive life cycle analysis with current production of plastics as a baseline
- Developing predictive environmental and toxicity modeling to inform new plastic recycling solutions, including plastics that can degrade in the environment or compost facilities
- Demonstrating systems analysis case studies for polymer recycling, including system-level techno-economic models to track secondary material flows to help identify and address inefficiencies in the recovery and processing of recyclables and increase the availability of secondary feedstocks.

# **PIC Research Directions**

Multiple research directions will be required to develop new technologies and gain scientific advances relating to the PIC. These directions represent key research areas that may help overcome the challenges facing each PIC goal area. Table 1 shows the interaction of research directions and the PIC goal areas. The key research directions include thermal processes to deconstruct plastics, chemical processes for deconstruction and creation of new materials, biological processes for deconstruction and creation of new materials, physical recycling and recovery to handle material processing and collection, and research that enables the design of new materials for circularity.

Although each of these research directions is listed separately, integrated research is critical to developing a comprehensive approach to tackle plastic waste. Thermal and biological processes may be combined so that biological organisms can upgrade the products of thermal degradation. Although chemical and biological processes are separated here to highlight the unique technological opportunities, almost every biological process will require a chemical process component. Likewise, chemical processes may often benefit from a biological component. Physical recycling and recovery will be required in thermal, chemical, and biological processes to collect and preprocess the material for deconstruction and upgrading. Similarly, a design for circularity will also underpin each of the other research development areas.

		Challenges	Thermal Processes	Chemical Processes	Biological Processes	Physical Recycling and Recovery	Design for Circularity
PIC Goals	Deconstruction	Retain value	٠	٠	٠	٠	٠
		Feedstock heterogeneity		٠	٠	٠	
		Contaminant removal	٠	•	•	٠	
		Multicomponent materials		٠	٠		٠
	Upcycling	Recover value		٠	•	٠	٠
		New material design		٠	•		٠
	Recyclable by Design	Design for reuse		٠	٠		•
		Compatibility with recycling infrastructure	•	٠	•	•	•
	Scale and Deploy	Life cycle assessment implications	•	•	•	•	•
		Management of distributed resource	•	•	•	•	•
		Circularity	•	•	•	•	•
		Scale of plastics challenge	•	•	•		•

#### Table 1. How PIC Goals Interact with Research Directions

**Research Directions** 

### **Thermal Processes**

Thermal processes nonselectively degrade plastics into an intermediate stream that can be further processed. For this roadmap, thermal processes that yield energy as the only product are not included, as the scope of the PIC seeks to move beyond energy generation. Some technologies considered here are gasification and pyrolysis. Gasification includes hydrogen and syngas production with subsequent upgrading. Pyrolysis technologies generate liquid fuel or upgradable intermediates from plastic.

Gasification and pyrolysis directly work toward the PIC goals. Relating to **deconstruction**, gasification and pyrolysis are uniquely suited to accept complex mixtures for deconstruction, as a complex polymer mixture is thermally degraded into syngas (H<sub>2</sub> and CO) or small hydrocarbon units, irrespective of the starting mixture. In comparison, a highly selective chemical or biological approach depends much more on the composition of the starting polymers. Gasification and pyrolysis are also suited for processing mixed materials, where a mixed-waste stream consisting of textiles or multilayer packaging are upgraded. Overall, thermal processes will directly face kinetic limits, as the reaction efficiency determines the scalability, energetic requirements, and cost of the process. R&D will be critical to optimize these deconstruction processes and to integrate these with subsequent upgrading.

Relating to the **scale-and-deploy** goal, the advantages of gasification and pyrolysis are underpinned by the life cycle implications. The benefit of degrading a plastic waste into a usable intermediate must outweigh other considerations such as process cost, energy input, water use, and any byproduct generation. Life cycle analysis will be critical to determine where thermal processes are advantageous. Finally, collection and sorting of the starting material and feedstock heterogeneity from a supply chain perspective are critical upstream considerations in developing a gasification or pyrolysis approach.

Opportunities for **upcycling** and new materials that are **recyclable by design** from thermal processes are possible if the intermediate stream generated can then be processed into a new material. One example here is the upgrading of plastic waste gasification-derived syngas through gas-fermenting microorganisms into a new plastic material. There are also opportunities for other chemical processes to incorporate thermal decomposition streams into new materials that may be upcycled or are designed for recyclability.

Thermal processes provide a unique route to process mixed and contaminated waste streams that are difficult to process using selective methods, but face the drawback of high energy intensity. Once the material is deconstructed thermally, many possibilities for recycling and upcycling exist, providing the incentive to convert existing plastic waste into new materials. New thermal processes are required to enable energy savings relative to plastic production from fossil sources, which is one of the Plastics Innovation Challenge metrics. In addition, these methods could provide efficient carbon conversion from waste plastic to upgradable intermediates and directly enable the overall progress toward a circular plastics life cycle. Some ongoing efforts may help develop transformative technologies.

# **Chemical Processes**

Chemical processes include catalytic or other chemical methods for polymer functionalization or degradation to an intermediate that may be upcycled, as well as chemical processes supporting new material design. Chemical processes for new material design include those that convert plastic and non-plastic feedstocks to new, recyclable, or biodegradable materials.

Chemical functionalization or degradation and subsequent upcycling connects to each of the PIC goals. From a **deconstruction** and material- and chemistry-based perspective, chemical processes hold great promise to selectively deconstruct existing plastic waste into upgradable intermediates of controlled composition. The feasibility of chemical degradation and upcycling intrinsically depends on the kinetics of the catalytic decomposition, the catalyst interaction with the polymer and its stability, and its ability to selectively degrade desired constituents in a complex mixture. Each of those areas poses a unique opportunity for research discoveries and technology development. The presence of contaminants poses a critical challenge facing chemical processes but may also provide an opportunity to use metals and other contaminant species to assist in separation or breakdown of the polymer. Chemical processes that are agnostic to composition or the presence of contaminants contain enormous potential to improve the processability of existing plastic waste but require substantial R&D advances before this type of approach is feasible.

Chemical processes foundationally contribute to the **upcycling** and **recyclable-by-design** goals. For upcycling, chemical processes may generate a specific and upgradable intermediate stream from depolymerized plastic waste, which facilitates the production of higher-value products. These new products derived from plastic waste may also be designed for recyclability by incorporating labile bonds in the polymer structure that will enable either future chemical recycling or biodegradation. Incorporating tags that enable sorting of the new material is another opportunity enabled by chemical processes. Materials that are designed for positive end-of-life outcomes, including recyclability or biodegradability, may also be produced from other renewable feedstocks beyond plastic waste. Because these new materials provide clear end-of-life and circularity benefits, new materials can be generated from renewable biomass-based or other waste feedstocks. DOE has a long history of converting renewable feedstocks into new materials. Here, new material design experience can be leveraged to produce new plastic materials that perform similarly or better than incumbent plastics and provide an end-of-life benefit. As with other research directions, understanding the life cycle implications of a chemical degradation and upcycling approach will be critical to understand the value proposition of the overall process beyond the direct process costs. The scale of the plastics market, as well as the volume of plastic waste, are both key variables that affect the types of technologies that may penetrate the plastic material and recycling markets. These considerations are critical to **scale and deploy** a chemical processing technology.

### **Biological Processes**

Similar to chemical processes, biological processes include both those that enable plastic deconstruction and those that enable the production of new plastic materials.

Biological processes benefit from the rich biosynthetic and biocatalytic diversity that has evolved over billions of years. Myriad catalytic pathways exist that have enabled microorganisms to break down and harness energy from otherwise recalcitrant material, often in extreme environments. Similarly, microorganisms have developed creative carbon-storage mechanisms by producing their own complex biopolymers. Due to this resourcefulness, microorganisms and the enzymes they produce confer unique advantages to tackling plastic waste. Biological processes may be uniquely suited to both degrading plastic waste and producing new materials that have desirable performance and end-of-life characteristics.

From a **deconstruction** perspective, microorganisms and their enzymes have shown promise in their ability to degrade plastic waste.<sup>27,28</sup> Despite the disadvantage of only a short evolutionary window in which microorganisms have coexisted with plastics, microorganisms' malleable metabolic networks have already adapted to consume some plastics. With additional evolutionary pressure in the laboratory, there is great promise to improve these existing degradation pathways, in addition to the development of novel pathways through enzyme engineering and laboratory evolution. The degradation of existing plastics or biodegradable plastics should be characterized to understand whether the material is completely degraded into benign products or if microplastics are generated as an unintended byproduct.

Microorganisms live in complex environments, often in the presence of what may be considered contaminants to catalysis processes. Biological processes may therefore enable the deconstruction of contaminated, mixed-plastic streams, where the contaminants may actually improve the microbial growth. In the cases where this contamination interferes with microbial growth, laboratory evolution may reduce the contaminant toxicity. There is an opportunity for biological processes to function at a wide range of temperatures and osmotic conditions, adding further to process integration feasibility of biological processes. The physical properties of nonpolar plastic polymers also pose a challenge to microbial degradation because these polymers must first interface with the microorganisms in their aqueous environment. Hybrid chemical-biological approaches may be employed to overcome this challenge.

The **upcycling** goal also benefits from the breadth of biological diversity. Biological processes may be tuned to produce tailored materials with desired functionality. Biological processes have long been employed to convert biomass feedstocks into biopolymers and complex, value-added chemicals. Converting plastic waste biologically into a valuable product represents an extension of a large body of bioengineering work that has been supported by DOE.

Biological processes also can directly address the **recyclable-by-design** goal. Biopolymers such as polyhydroxyalkanoates are produced naturally by bacteria and are naturally biodegradable, and therefore biologically recyclable (i.e., other microorganisms can naturally degrade and recycle these materials). Beyond naturally recyclable biopolymers, biological processes can be leveraged to produce new plastics that are

 <sup>&</sup>lt;sup>27</sup> Dominik Danso, Jennifer Chow, and Wolfgang R. Streit. 2019. "Plastics: Environmental and Biotechnological Perspectives on Microbial Degradation." *Applied and Environmental Microbiology* 85(19): e01095-19. https://doi.org/10.1128/AEM.01095-19.
<sup>28</sup> Jiakang Ru, Yixin Huo, and Yu Yang. 2020. "Microbial Degradation and Valorization of Plastic Wastes." *Frontiers in Microbiology* 11.

<sup>&</sup>lt;sup>28</sup> Jiakang Ru, Yixin Huo, and Yu Yang. 2020. "Microbial Degradation and Valorization of Plastic Wastes." Frontiers in Microbiology 11. https://doi.org/10.3389/fmicb.2020.00442.

designed to be recyclable, either biologically or chemically. Again, microorganisms can be adapted and engineered, leveraging biosynthetic diversity, to produce desired polymers or polymer precursors.

The **scale-and-deploy** goal is important to consider as it relates to biological processes. Although biology confers significant advantages, extensive work will be required to reduce the cost of many biological processes. The scale of plastic production and plastic waste also must be considered when developing a biological process.

# **Physical Recycling and Recovery**

Physical recycling and recovery are intimately tied to the goals to improve **deconstruction** and essential to consider in new materials that are **upcycled** or **recyclable by design** in a **scalable and deployable** manner. One of the key challenges facing upgrading of plastic waste is its heterogeneity, including contaminants that can devalue potential recycling streams. To process and upgrade these materials, sorting and separations of valuable components from contaminants are critical. Sorting technologies intrinsically consider material properties to reduce the complexity of feedstocks for downstream processes. Sorting further addresses each of the application-based challenges by removing contaminants. From an application perspective, mixed materials are a subcategory of a complex feedstock, including such materials as multilayer packaging or textiles, where the single material is not homogeneous. Sorting technologies may help break these mixed materials down into usable components. Sorting also affects design for reuse. As new technologies are designed for reuse or improved recyclability, it will be critical to isolate these new materials. The sorting of these materials therefore connects directly with retaining the value of both existing plastic waste and new plastic materials. Finally, from a supply-chain perspective, separations and sorting are key considerations for any life cycle assessment and critical for managing a distributed, heterogeneous resource.

Mechanical recycling is the most common method of recycling today. It is an economical and energy-efficient pathway to convert waste plastic to usable material. However, it generally degrades the plastic, leading to worse mechanical properties and limiting the extent to which it can be used in future applications and the number of cycles the material can go through. Improvements to mechanical methods and utilizing mechanical methods in conjunction with other methods (e.g., chemical, biological) could lead to low-energy, economical pathways for recycling plastics.

### **Design for Circularity**

The novel or advanced recycling techniques discussed previously are crucial to begin addressing the global plastic waste challenge, but a permanent solution will be realized only when high-volume commercial plastics are designed for circularity. Significant work is required in this research area to meet the PIC **deconstruction** goal. Progress in developing scalable thermal, chemical, and biological processes to deconstruct polymers back into monomers or other valuable chemical intermediates is providing fresh insights into designing new chemistry and properties into plastics for circularity. This redesign will include solutions that are complementary to as well as independent from advanced recycling techniques, as new materials will need recycling solutions that preserve or enhance their waste value. These research directions may therefore advance the **upcycling** and **recyclable-by-design** PIC goals.

To be effective in closing the loop on plastics recycling, design-for-circularity technology must define an integrated set of processes for the entire circular life cycle. Processes for polymerization and manufacturing, collection and sorting, controlled deconstruction and purification, and reconstruction to new plastics must work together to be energy-efficient with minimal life cycle costs. Circular plastics technology must be fully compatible with plastics manufacturing and feedstock requirements, recycling infrastructure, the inherent heterogeneity of most plastic waste, and the scale of the plastics industry, and any leaked materials from these processes will need to be designed to degrade or persist in durable materials. Though there is a heavy materials chemistry angle in designing for circularity, this research area touches on every other technology that improves the value and recyclability of plastic waste and needs to address major challenges within all four goals of the PIC.

The design for circularity of commodity polymers is an incredible challenge. A key consideration for **deconstruction** includes the stability of the saturated carbon-carbon bonds found in a large majority of commodity plastics. Gasification of plastic waste produces chemical building blocks in the form of syngas that can be used to reconstruct polymers in a circular fashion, and polymer deconstruction followed by repolymerization is possible for a few plastics like polyethylene terephthalate. However, these materials need to be **recyclable by design**. These future polymers designed for circularity will likely feature labile functional groups, such as esters, carbonates, and certain ethers, that allow for straightforward and selective depolymerization to yield high-purity monomers for chemical recycling. Ensuring that these new materials match the required properties of previous materials while also being cost-competitive is the only way to enable their adoption.

Consequently, in addition to the redesign of polymers for circularity, there is also opportunity to redesign the infrastructure around polymer recycling to improve circularity. Improved thermomechanical recycling techniques that prevent polymer molecular weight and property degradation will allow for modern, non-deconstructable polymers to greatly improve their circularity. Improved sorting and waste retention also decrease material leakage and further improve this circularity. Circularity may also be achieved through compatibilization of plastic waste to a useable polymer feedstock, reactive separation of the valuable components of mixed plastics, and selective **deconstruction** of polymers to chemical intermediates that are specifically designed for another application post-use. Intelligent material design with a robust understanding of post-use feedstock and remanufacturing opportunities and their applicable markets is the crux of **upcycling** and a way to improve both circularity and the value proposition of a new material.

Both the energy efficiency and carbon utilization of the circular process design are important. Designing such materials to be biologically or environmentally degradable on reasonable time scales, should leakage into the environment occur, will be critical for a holistic solution to plastic waste. Developing options for sourcing the monomers for such materials from bio-renewable resources further adds to the circular aspect of the overall design.

### **Research Activities and PIC Metrics**

Efforts in these research directions are essential to meet the PIC goals and metrics. To meet the metric to provide greater than 50% energy savings compared to virgin plastic production, advances will be required in each of the PIC goal areas through efforts in each research direction. Similarly, to achieve the targeted  $\geq$ 75% carbon utilization from waste plastics, significant advances will be required in each PIC goal area. Deconstruction advances will be critical, but the metrics will be impossible to meet without simultaneous advances, such as scaling and deploying nascent technologies. Likewise, advances in chemical processes will depend heavily on advances in the circularity and physical processing research areas. There are many research opportunities that may contribute to achieving the PIC metrics while providing an improved scientific understanding of polymer decomposition and design.

# **DOE Activities**

DOE activities have begun to tackle some of the considerable R&D hurdles facing the PIC goals. Ongoing activities integrally connect with future work that will help develop innovative technical solutions to reduce existing plastic waste, as well as to develop new materials with improved end-of-life properties. The activities listed here span current work that has recently begun, as well as future activities for DOE investment.

# **Thermal Processes**

#### Fundamental

• Gain a mechanistic understanding of thermal depolymerization processes

- Understand and control reaction pathways for gasification and pyrolysis of plastics through deciphering the chemical mechanisms in complex thermal processes
- The mechanistic understanding of polymer pyrolysis can be used to control the synthesis of valueadded materials
- Enhance thermal depolymerization of plastics in gas-phase or liquid processes through pulsed thermolysis to interrogate the impact of impurities and additives on the breakdown of mixed feedstock streams
- Couple thermal methods with catalytic and biological methods for funneling mixtures and fundamental building blocks, like those produced from thermal degradation of plastics, into a useable distribution of valuable products.

#### Applied

- Develop alternative materials and processes to expensive superalloys and refractories to avoid corrosion that occurs during gasification and understand the impact of plastics as a feedstock for the production of gases that can then be recycled or upcycled
- Assess the impacts on gasification processes and syngas composition from blending plastics with coal and/or biomass to produce net-zero-carbon, or even carbon-negative, products
- Reduce the cost and improve efficiency of thermal processes to gas and liquid intermediates that can be recycled or upcycled in a sustainable manner.

#### **Chemical Processes**

#### Fundamental

- Design new selective catalysts to control the reaction mechanisms of chemical deconstruction and upcycling of plastics. Research will include:
  - Experimental and computational studies of reaction mechanisms and novel tools and characterization strategies to probe and unravel the mechanisms, including at centers such as the Energy Frontier Research Centers.
- Explore nonthermal methods of polymer deconstruction, including electro-mediated processes that extend beyond current methods, which rely primarily on hydrogenolysis or oxidizing thermal conditions
- Develop selective polymer functionalization, which may offer the potential for dynamic or reactive separation strategies to be applied toward the challenge of mixed feedstock streams.

#### **Chemical Processes at the Energy Frontier Research Centers**

This research will build upon transdisciplinary research supported in the Energy Frontier Research Centers, as well as smaller efforts targeted at advancing polymer deconstruction strategies that access new higher-value monomers from polyolefins.

#### Applied

• Explore process improvements within existing chemical manufacturing industry to reduce the cost and improve the efficiency of these process such that there is a value proposition that will ultimately reduce plastic waste generation

• The Bio-Optimized Technologies to keep Thermoplastics out of Landfills and the Environment (BOTTLE<sup>TM</sup>) National Laboratory-led consortium (www.bottle.org) continues to optimize and intensify chemical methods to deconstruct and upcycle plastics, relying on fundamental science breakthroughs that have enabled carbon-carbon bond cleavage.

# **Biological Processes**

#### Fundamental

- Understand the molecular mechanisms for enzymatic deconstruction of plastics to provide input into metabolic pathways and inform the design of both new biosynthetic pathways in organisms and synthetic catalysts
- Leverage biological phenomena to identify, develop, and potentially design novel biological mechanisms, enzymes, and pathways to deconstruct and convert plastic polymers into a diverse range of products
- Extend the foundational knowledge on lignocellulose biomass deconstruction, including efforts at the Bioenergy Research Centers, to other macromolecular transformations such as plastic polymers
- Invest in advances in genomic science, synthetic biology, and computational biology to broaden available opportunities to design plants and microorganisms for the purpose of producing novel plastic materials with enhanced capabilities or to substantially reduce their environmental impact.

#### Applied

- Invest in energy- and carbon-efficient biological manufacturing pathways for a variety of applications
- Explore enzyme optimization and systems engineering biological processing to develop environmentally friendly recycling technologies for current and future plastics.

#### **Breakthroughs for Biological Plastics Recycling**

The recent discovery and optimization of enzymes capable of breaking down some plastics like PET into its constituent monomers has opened the door to new ways of thinking about recycling.

# **Physical Recycling and Recovery**

#### Fundamental

- Gain basic advances in sorting technologies and polymer composition to improve physical recycling and recovery
- Develop models to reflect material flows and end-of-life fate.

#### Applied

- Through efforts within the REMADE Institute, optimize mechanical and chemical recycling processes
- Develop effective sorting and cleaning of secondary plastics feedstocks and contaminant removal
- Develop methods to cost-effectively compound recycled plastics into primary plastics.

#### Physical Recycling and Recovery at the REMADE Institute

The REMADE Institute is focused on accelerating physical recycling through technological solutions in five key areas: Systems Analysis and Integration, Design for Re-X, Manufacturing Materials Optimization, Remanufacturing and End-of-Life Reuse, and Recycling and Recovery.

# **Design for Circularity**

#### Fundamental

- Enable precision cleavage of polymers into lower-molecular-weight molecules suitable for material applications (e.g., industrial and motor lubricants)
- Explore a range of new circular chemistries, including ring-opening polymerization with ring-closing depolymerization, cyclopolymerization with retro-cyclodepolymerization, supramolecular bond-forming polymerization with supramolecular bond-breaking depolymerization, and other chemistries with similar reversible outcomes
- Design efforts to replace thermosetting polymers by focusing on developing similar reversible chemistry for the cross-links that can be triggered by a stimulus (e.g., heat, electrochemical, sonication) that is not present in the normal operational environment for the material.

#### Applied

- Develop bio-based and biodegradable polyurethanes, as well as polycarbonate vitrimers, to be used in thermosets and upcycled into solvents for battery technologies (BOTTLE)
- Investigate the redesign of multilayer packaging materials through bio-based novel polyesters, which are expected to demonstrate improved biodegradability
- Design plastics to be more recyclable or biologically degradable (BOTTLE Funding Opportunity Announcement, the BOTTLE Consortium, and the REMADE Institute)
- Continue efforts to design multicomponent products such as batteries, electronics, and composites to be more easily recycled, repaired, and reused (ReCell, Institute for Advanced Composites Manufacturing Innovation, and REMADE Institute).

### **BOTTLE Consortium**

Supported by both the Bioenergy Technologies Office and the Advanced Manufacturing Office, BOTTLE is a multi-organization consortium focused on developing new chemical upcycling strategies for today's plastics and creating tomorrow's plastics to be recyclable by design. BOTTLE's vision is to deliver selective, scalable technologies to enable cost-effective recycling, upcycling, and increased energy efficiency.

### ReCell

The ReCell Center, a lithium-ion battery recycling center at Argonne National Lab, is focused on innovative cost-effective recycling processes to make lithium-ion recycling profitable for current and next-generation lithium batteries. ReCell conducts research in four areas including direct recycling and upcycling of cathodes, recovery of other materials like graphite and electrolytes, modeling and analysis

focused on techno-economic modeling and materials characterization and qualification, and design for sustainability to transition to cell and battery design with reuse and recycling in mind.

#### Institute for Advanced Composites Manufacturing Innovation

The Institute for Advanced Composites Manufacturing Innovation (IACMI) is a public/private partnership validating manufacturing technologies that respond to private industry's need for faster and more cost-, material-, and energy-efficient composite manufacturing, including recycling at the end of product life.

# **DOE Capabilities and Coordination**

The U.S. Department of Energy supports a broad range of capabilities in fundamental and applied research. This includes a network of user facilities and coordinated R&D efforts to ensure rapid innovation and progress in a variety of technology areas. The Plastics Innovation Challenge has effectively brought together a large number of these capabilities to tackle plastic waste through a coordinated R&D approach.

### Coordination

Research efforts are coordinated by regularly scheduled coordination meetings, including discussions on recently funded research, impactful research outcomes, upcoming funding opportunity announcements (FOAs), and new scientific and technical challenges. Joint FOA and Small Business Innovation Research (SBIR) opportunities have been hosted to establish direct coordination between offices, specifically the joint BOTTLE FOA sponsored by BETO and AMO. Coordination of FOA development between offices will also continue. Beyond competitive funding opportunities, institutes and consortia contribute focused and continuous capabilities. Some of the key DOE organizations that support PIC efforts include the BOTTLE Consortium, the REMADE Institute, ReCell Center, the Institute for Advanced Composites Manufacturing Innovation, and the Energy Frontier Research Centers. Coordination also occurs between DOE and other agencies regarding PIC efforts, including the National Science Foundation, the National Institute for Standards and Technology, the U.S. Department of Agriculture, and the U.S. Environmental Protection Agency.

Feedback from stakeholders, as described in the Challenges and Opportunities section, is regularly solicited to ensure efforts are reflecting recent R&D advancements and industry needs. Future workshops, webinars, and joint conference sessions will be planned and coordinated to ensure that investigators from various offices maintain communication, coordination, and collaboration.

This approach establishes a robust pipeline of fundamental science innovation that can then be optimized and refined to create economically viable and environmentally friendly solutions to the problem of plastic waste. The offices that have directly contributed to this effort, as well as their capabilities and contributions, are described here. The capabilities listed below are considered heavily when coordinating research efforts across offices.

### **Office of Science**

The Office of Science supports research that probes the frontiers of physics, chemistry, materials science, and systems biology. It is the steward of 10 of the 17 DOE National Laboratories, which house world-leading scientific user facilities including five X-ray light sources, two neutron scattering facilities, five Nanoscale Science Research Centers, the Joint Genome Institute (JGI), and the Environmental Molecular Sciences Laboratory (EMSL), as well as world-leading high-performance computing facilities and computational infrastructure, including the DOE Systems Biology Knowledgebase (KBase) computational platform. Within the Office of Science, two programs support research relevant to PIC—BES and BER.

#### **Basic Energy Sciences**

BES supports fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels. BES research relevant to PIC includes novel catalyst design and quantum- and molecular-level control of chemical transformations; the understanding of reaction mechanisms, enabling precise identification and manipulation of catalytic active sites, their environments, and reaction conditions for optimized efficiency and selectivity; studies of active-site protein chemistry that provide a basis for highly selective and efficient bio-inspired catalysts; and design and synthesis of novel materials with an emphasis on the chemistry and chemical control of structure and collective properties.

#### **Biological and Environmental Research**

BER supports research on biological systems to identify the foundational principles that govern biological systems to understand, predict, manipulate, and design biological processes that underpin innovations for bioenergy and bioproduct production, as well as to enhance the understanding of natural environmental processes. BER's currently funded research portfolio consists of numerous areas relevant to PIC, including genomic and microbiome science to explore biological mechanisms for polymer breakdown and conversion; identification and/or modifications of metabolic pathways, organisms, and microbial communities to convert polymers to value-added bioproducts; and computational resources and novel analysis tools to leverage systems biology data for genome editing to design new biological systems.

# Office of Energy Efficiency and Renewable Energy

DOE's Office of Energy Efficiency and Renewable Energy (EERE) seeks to create and sustain American leadership in the transition to a global clean energy economy. Two EERE programs—the Advanced Manufacturing Office and Bioenergy Technologies Office—coordinate with other DOE offices to support the PIC.

#### **Advanced Manufacturing Office**

AMO develops technologies that reduce direct and life cycle energy demands, drive energy productivity improvements in the U.S. manufacturing sector, efficiently utilize abundant and available domestic energy resources, and support the manufacture of clean energy products, with benefits extending across the economy. Through previous and current investments in the circular economy, AMO has conducted analysis and developed tools to guide future investment and quantify life cycle benefits of work in the PIC. Strong connections with industry partners throughout the recycling supply chain have been established through consortia, R&D projects, and the Better Plants program that can be leveraged to scale and deploy technology developed.

#### **Bioenergy Technologies Office**

BETO develops and demonstrates transformative and revolutionary sustainable bioenergy technologies for a prosperous nation. One current focus of BETO is the utilization of waste resources such as agricultural residues, organic wastes, and municipal solid waste—including plastic—to make high-value bioproducts and biofuels. Capabilities developed to deconstruct and upgrade these waste resources are utilized in the Plastics Innovation Challenge to provide novel routes to plastic upcycling as well as redesign of plastics from biologically derived sources. Key to these activities is a focus on process techno-economics and life cycle emissions, ensuring development of economically viable and environmentally friendly technologies.

# **Office of Fossil Energy**

The Office of Fossil Energy is responsible for federal research, development, and demonstration efforts on advanced power generation and polygeneration; power plant efficiency; water management; coal to products; critical minerals; carbon capture, utilization, and storage technologies; and emission-control technologies, as well as the development of technological solutions for the prudent and sustainable development of our unconventional oil and gas domestic resources. The gasification, pyrolysis, and CO<sub>2</sub> utilization programs have been working for decades on associated technologies that can be used for thermochemical conversion to gasify

co-fired plastics for syngas, hydrogen, and CO<sub>2</sub> as the building blocks for valuable materials. The programs are working with industry stakeholders to develop advanced gasification processes and utilize CO<sub>2</sub> to form new polymers or building blocks for new plastics. The program also integrates carbon capture, utilization, and storage into all systems to reduce carbon and other emissions.

# Advanced Research Projects Agency-Energy (ARPA-E)

ARPA-E's mission is to decrease our nation's dependence on foreign energy sources, reduce greenhouse gas emissions, improve energy efficiency across the board, and maintain or reestablish U.S. scientific leadership in the energy sector. ARPA-E awarded four contracts in 2020 for "Recycle Underutilized Solids to Energy (REUSE),"<sup>29</sup> an exploratory program to develop technologies that convert unrecycled plastics and/or paper to a high-energy-content liquid product that can be used for refinery or chemical feedstocks, or directly for fuel. The goal is to identify processes that could be deployed economically at the scale of 100–500 tons per day.

# **PIC Research Timeline**

Near-, medium-, and long-term R&D priorities have been identified that will help guide DOE's work on the PIC goals. Figure 4 shows a progression of this work in both fundamental and applied areas. The four selected challenges represent the key challenges facing each of the PIC goal areas.

<sup>&</sup>lt;sup>29</sup> https://arpa-e.energy.gov/technologies/publications/white-paper-background-information-arpa-es-reuse-program.



# DECONSTRUCTION

- Advance developments in thermal depolymerization in gas or liquid-phase processes.
- Design new selective catalysts to control reaction mechanisms of chemical deconstruction of plastics.
- Develop robust methods for biological and chemical deconstruction of mixed plastic waste, with an understanding of the molecular mechanisms.

# UPCYCLING

- Target upcycling applications for materials that can be deconstructed today, such as PET.
- Couple deconstruction methods with selective upcycling pathways that ultimately convert plastic waste to high-value materials.
- Combine selective deconstruction and upcycling using catalytic and biological methods of funneling breakdown intermediates into valuable products.

# **RECYCLABLE BY DESIGN**

- Broaden opportunities to design organisms for the purpose of producing novel plastic materials using a confluence of advances in genomic science, synthetic biology, and computational biology.
- Develop new chemistry to enable materials to be recyclable by design, including leveraging polymer chemistries susceptible to selective depolymerization under specific conditions.
- Design multicomponent products engineered for recyclability, repair, and reuse, such as batteries, electronics, and composites.

# **SCALE AND DEPLOY**

- Establish and implement contaminant removal and effective sorting of secondary, mixed-plastic feedstocks.
- Develop basic advances in sorting technologies and polymer composition to improve physical recycling and recovery.
- Advance biological systems for environmentally friendly recycling technologies for current and future plastics.

Figure 4. Timeline of how R&D investments address identified challenges in the near, medium, or long term

# Conclusion

Plastic waste presents both an opportunity to achieve superior economic and environmental outcomes as well as a technological challenge to develop new processes and materials. The Plastics Innovation Challenge and DOE are uniquely suited to transform the landscape of plastic materials and plastic waste. This roadmap describes the path toward significant technology development, with the potential to meet each of the PIC goals. The key actions for each of the goals are summarized here.

# **Deconstruction**

- 1. Develop deconstruction methods that leverage chemical, biological, and thermal approaches for both selective and nonselective deconstruction. Developing technologies in each of these research areas will collectively improve the capacity to handle all types of plastic waste, and hybrid approaches are likely essential.
- 2. Develop deconstruction processes to characterize and overcome challenges with dispersed, heterogeneous, multi-material, and contaminated plastic waste streams.

# Upcycling

- 1. Identify and develop new strategies for upcycling, which are essential for converting waste plastic into valuable new materials. Upcycling will enhance the value of plastic waste and create a stronger economic incentive for material and energy recovery from plastics.
- 2. Develop deconstruction methods coupled with selective upcycling pathways that ultimately convert challenging plastic feedstocks to high-value materials. This will rely on novel catalytic and biological methods for funneling mixtures of fundamental building blocks, like those produced from thermal degradation of plastics, into a useable slate of valuable products.
- 3. Identify and develop markets for upcycled materials that maximize the economic and environmental value of the input materials.

# **Recyclable by Design**

- 1. Utilize advances in genomic science, synthetic biology, and computational biology to design biological systems for the purpose of producing novel plastic materials with advantaged properties and superior end-of-life options.
- 2. Co-design new polymeric materials for desired properties and the chemical mechanisms for their efficient deconstruction and assemble into desired products, enabling the development of plastics that are recyclable or biodegradable by design with properties that exceed incumbent materials.

### **Scale and Deploy**

- 1. Develop specifications for mixed-plastic waste to allow recyclers to process waste in the most economically and environmentally efficient way possible.
- 2. Improve collection and sorting technologies to enable larger amounts of plastics to be collected for processing and enable those plastics to be more easily recycled or upcycled.
- 3. Improve frameworks for assessing energy and environmental impacts of plastics during their manufacturing and end of life.
- 4. Demonstrate technologies at relevant scales with real-world feedstocks to de-risk development and deployment by industry.

This roadmap outlines a path along which DOE may leverage its existing infrastructure to meet the goals of the PIC.





For more information, visit: energy.gov/plastics-innovation-challenge

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