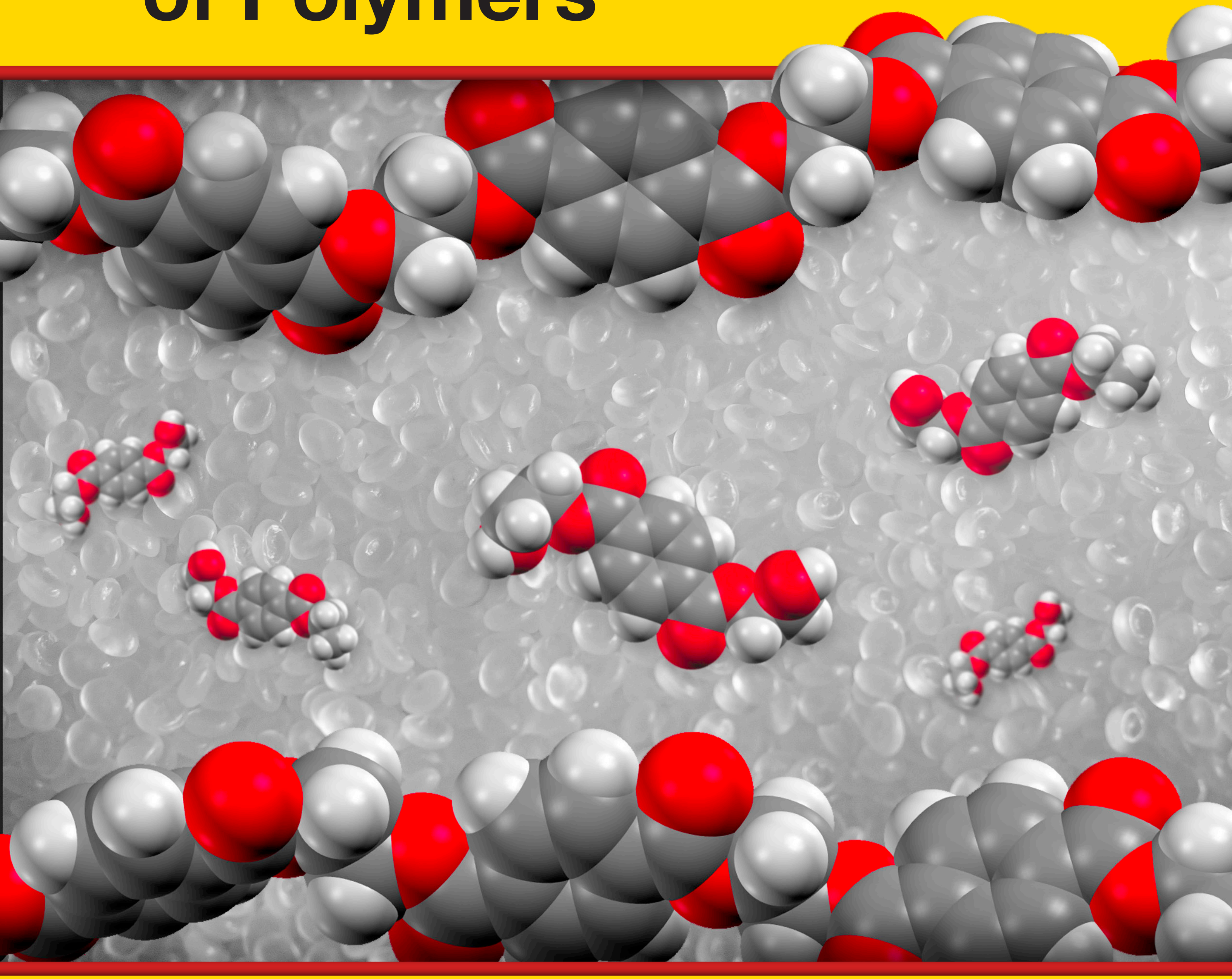
Roundtable on

Chemical Upcycling of Polymers



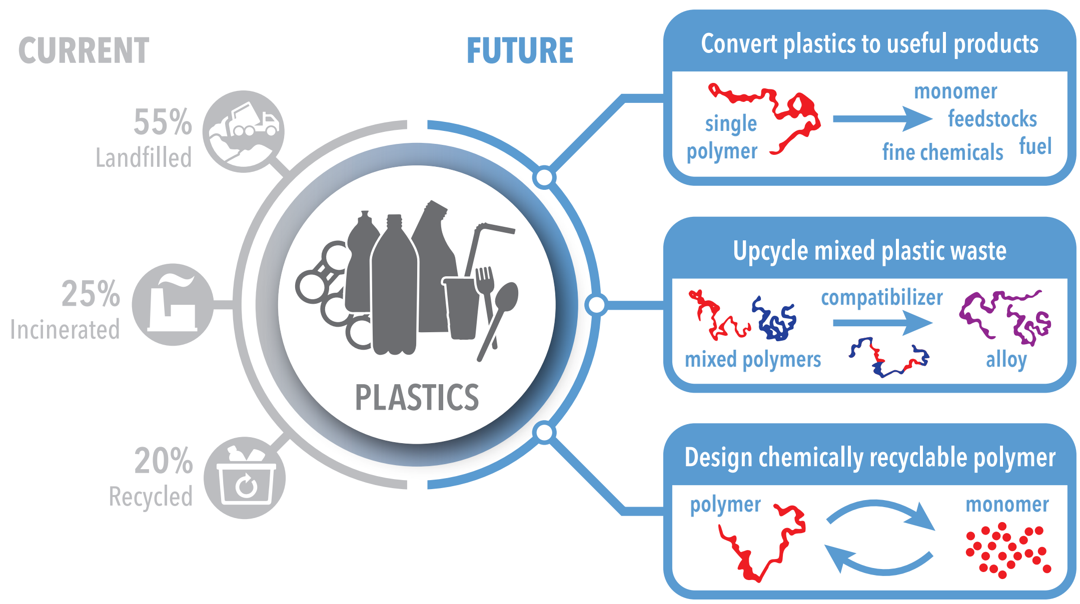
Revolutionizing the lifecycle of plastics

Chemical Upcycling of Polymers—Transforming discarded plastic from waste to high-value products

Plastics are ubiquitous in modern life. They are made from synthetic carbon-based polymers—organic macromolecules made up of many repeating subunits called monomers—and are designed to be durable and resistant to degradation. Global plastics production has reached a rate of over 400 million metric tons per year, with over 8 billion metric tons produced in the past 50 years. Average production has increased by 36% in the past decade and is projected to grow to 700 million metric tons in 2030—about 80 kg of plastics produced for every human on earth. Globally, 20% of discarded plastics are recycled (<10% in the United States), primarily using mechanical processes, and about 25% are incinerated for energy recovery. More than half are deposited into landfills or released into the environment. Thus, plastic waste poses a long-term environmental challenge: e.g., at the current rate of plastics production and disposal, the mass of plastic waste in the ocean is predicted to exceed the mass of fish by 2050.

Plastics represent a resource for making chemicals, fuels, and materials. Although incineration eliminates wastes and recovers some of the energy used to make the plastic, it uses up the potential resource and creates unwanted byproducts. Mechanical recycling—which involves shredding, heating, and remolding of the plastics—is more efficient than making them from petroleum products, using less than half as much energy to generate new plastics. However, mechanical recycling degrades, or downcycles, the polymers. Chemical recycling deconstructs polymers to produce molecular intermediates that can be used as building blocks to make new products, offering the opportunity to turn discarded plastics into higher-valued products. However, current approaches (e.g., pyrolysis—high-temperature processing in the absence of oxygen), are energy-intensive and require further processing to make products. Polymer upcycling represents a new approach: selectively deconstruct polymers into chemicals, fuels, or molecular intermediates and couple the deconstruction with reconstruction of these intermediates into high-value products under mild conditions. A significant opportunity exists for fundamental research to provide the foundational knowledge required to enable polymer upcycling, which holds the promise of changing the paradigm for discarded plastic from waste to valued resource by moving to a circular lifecycle for plastics.

Basic Energy Sciences held a Roundtable on Chemical Upcycling of Polymers in April 2019 to identify the fundamental challenges and research opportunities that could transform discarded plastics to higher-value fuels, chemicals, and materials. Four Priority Research Opportunities were identified to address the complex chemical transformations and physical processes underlying the upcycling of discarded plastics. The full report will be available at https://science.osti.gov/bes/Community-Resources/Reports.



Priority Research Opportunities

- **Master the mechanisms of polymer deconstruction, reconstruction, and functionalization**
  Key question: *How do we develop selective and integrated chemical processes to upgrade a discarded plastic into a desirable product?*
  The chemical stability and physical properties that make plastics valuable for various applications also make their selective chemical conversion to new products a grand challenge. Existing methods to transform the macromolecular structures of plastic are nonselective and energy intensive. New energy-efficient catalysts, macromolecular transformations, and chemical processes are needed to selectively deconstruct polymer chains in a discarded plastic into intermediates that can be reconstructed into desirable products (e.g., chemicals, fuels, or new polymers), or directly convert discarded plastics into materials with new functions.

- **Understand and discover integrated processes to upcycle mixed plastics**
  Key question: *How can we directly transform mixed discarded plastics to desirable products?*
  Many plastic products are made from multiple polymers and contain additives (such as pigments and stabilizers), fillers, and residues. Physical separation of these complex mixtures to recover pure components is technically challenging. This presents an opportunity to develop new energy-efficient integrated chemical, catalytic, and separations approaches that address the chemical and physical challenges of mixed plastics and directly capitalize on their chemical complexity. These efforts will allow the transformation of mixed plastics to chemicals and fuels, as well as to new materials.

- **Design next-generation polymers for chemical circularity**
  Key question: *How can we design new polymers that have the properties of today's polymers and enable simple reuse of the molecular building blocks?*
  Except for polyethylene terephthalate, commercial plastics are generally not recycled in a closed-loop, circular manner, in part because methods to selectively deconstruct polymers back to their original monomers are absent. New plastics need to be intentionally designed for the desired properties and chemical circularity at the molecular level with the goal of closing the loop in plastics recycling and chemical upcycling. New monomer and polymer chemistries need to be developed that both deliver next-generation polymers with properties similar or superior to those of current polymers and enable circular lifecycles using atom- and energy-efficient processes.

- **Develop novel tools to discover and control chemical mechanisms for macromolecular transformations**
  Key question: *What experimental and computational tools are needed to elucidate the macromolecular transformations of plastics in complex, nonequilibrium media?*
  Deconstruction and reconstruction of polymers involves complex coupling of chemical and physical processes that span a wide range of length and time scales. This inherent complexity demands a new paradigm that integrates advanced experiments and computation. When in situ and operando characterization methods are coupled with real-time computational modeling, simulations, and data analytics, the mechanisms and kinetics of deconstruction, reconstruction, and separations will be uncovered. These advanced multifaceted techniques will produce predictive insights into the design of new chemical transformations and processes for converting discarded plastics to desired products.

Summary

Chemical upcycling of discarded plastics to higher-value fuels, chemicals, or materials will revolutionize the lifecycle of plastics while saving energy and reducing the environmental impact of plastics. Advances in the Priority Research Opportunities identified in this report will provide the foundational knowledge needed to design new chemical reactions, catalysts, processes, and materials that enable efficient deconstruction, reconstruction, and functionalization of discarded plastics into high-value products. Mechanistic insights gained from the deconstruction of a pure polymer will be used to develop new approaches and processes for deconstruction of mixed polymer streams. Integration of deconstruction and reconstruction schemes will provide unprecedented opportunities for the creation of new polymers to extend the useful life of discarded plastics. New monomers and polymers will be designed and synthesized that will exhibit chemical circularity; and currently nonrecyclable polymers, such as thermosets, will be recyclable through the design of new reversible chemical reactions. These advances will require the integration of precise synthesis with detailed mechanistic studies using real-time characterization and analysis tools coupled to computational modeling, theory, and data science tools. Through fundamental research into the chemical upcycling of polymers, a new paradigm will emerge in which discarded plastic is captured and becomes a resource, enabling efficient production of high-value chemicals, fuels and new polymeric materials and reducing the accumulation of plastic wastes in the environment. In addition, chemical upcycling will shift the raw material for making polymers from fossil fuels, which is predicted to consume as much as 20% of the world's oil production in 2050, to discarded plastics.

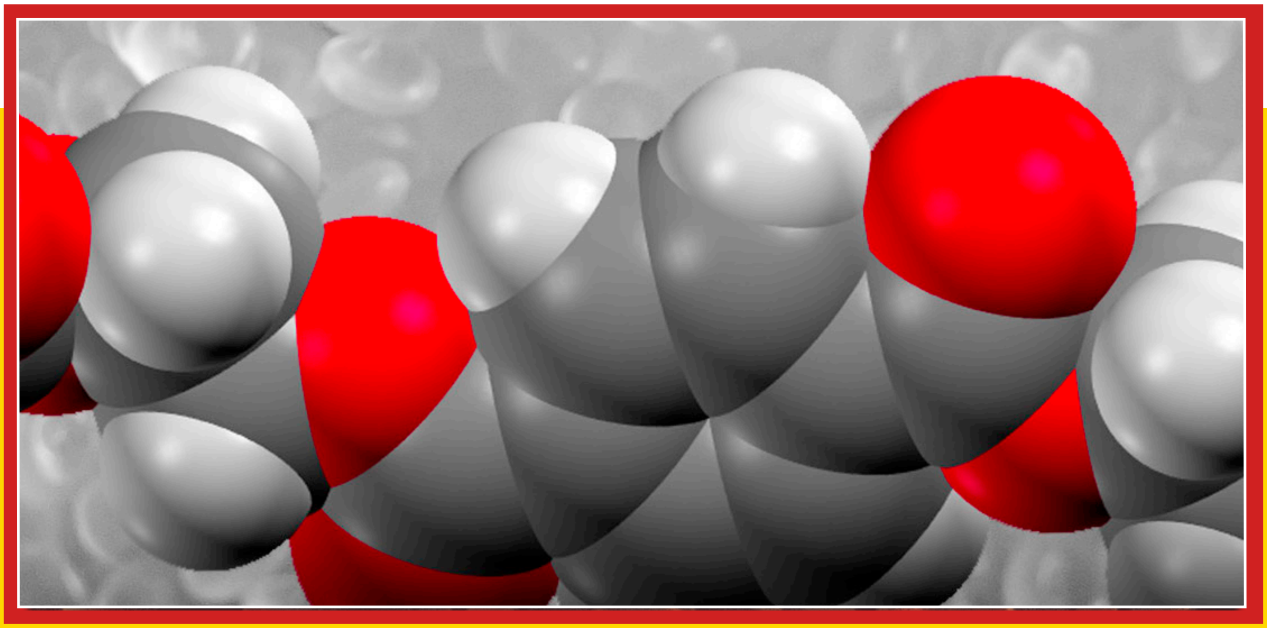


Image courtesy of Oak Ridge National Laboratory.

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