U.S. DEPARTMENT OF ENERGY | Office of Science

# Roundtable on Chemical Upcycling of Polymers

## Briefing to BESAC

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Oak Ridge National Laboratory
March 8, 2018

# BES Roundtable on Chemical Upcycling of Polymers

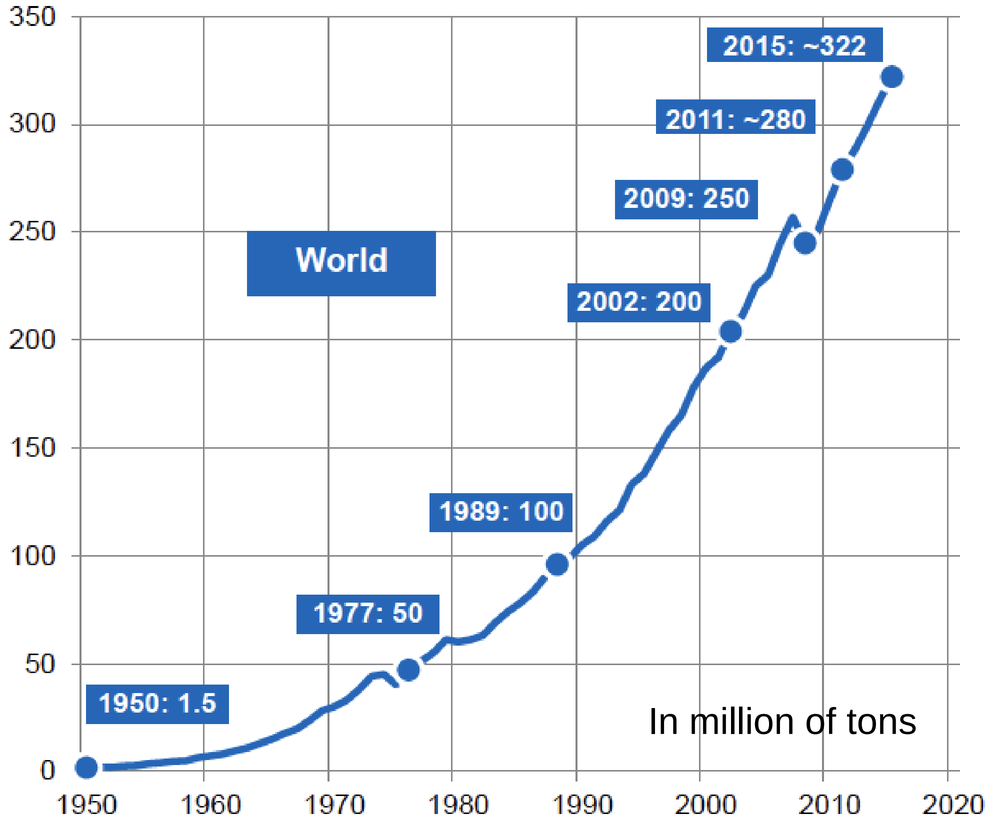
Workshop Chair: Phillip Britt (ORNL)
Co-Chairs: Geoff Coates (Cornell Univ.)
Karen Winey (Univ. of Penn.)
SC Technical Lead: Bruce Garrett

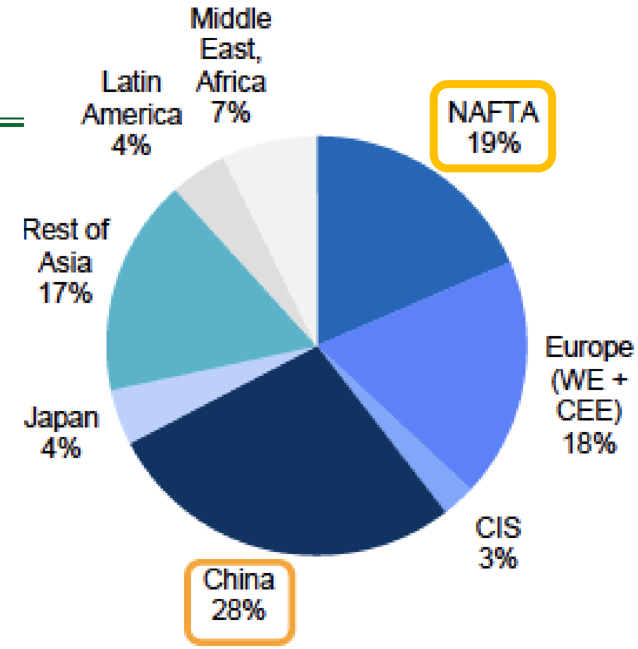


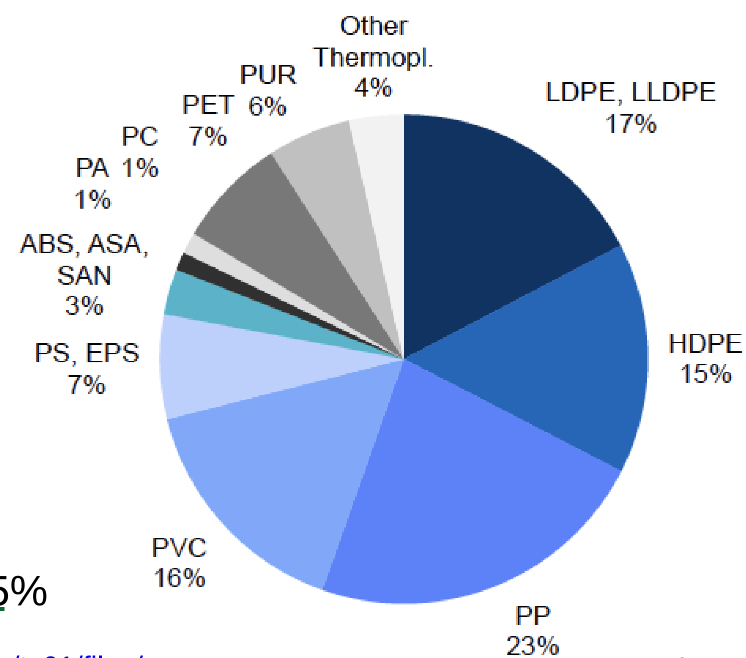
## Charge:

- Assess the fundamental challenges that would enable transformation of discarded plastics to higher value fuels, chemicals, or materials
- Identify fundamental research opportunities in chemical, materials, and biological sciences that will provide foundational knowledge leading to efficient, low-temperature conversion of discarded plastics to high-value chemicals, fuels, or materials
- Identify research opportunities for the design of new polymeric materials for efficient conversion, after end of life, to high-value chemicals or materials

# Globally Plastics are Growing




- If plastic production continues its current growth rate, then the plastics industry may account for 20% of the world's total oil consumption
- In 2015, global plastic waste disposal
  – Discard: 55%; Recycle: 19.5 %; Incineration: 25.5%

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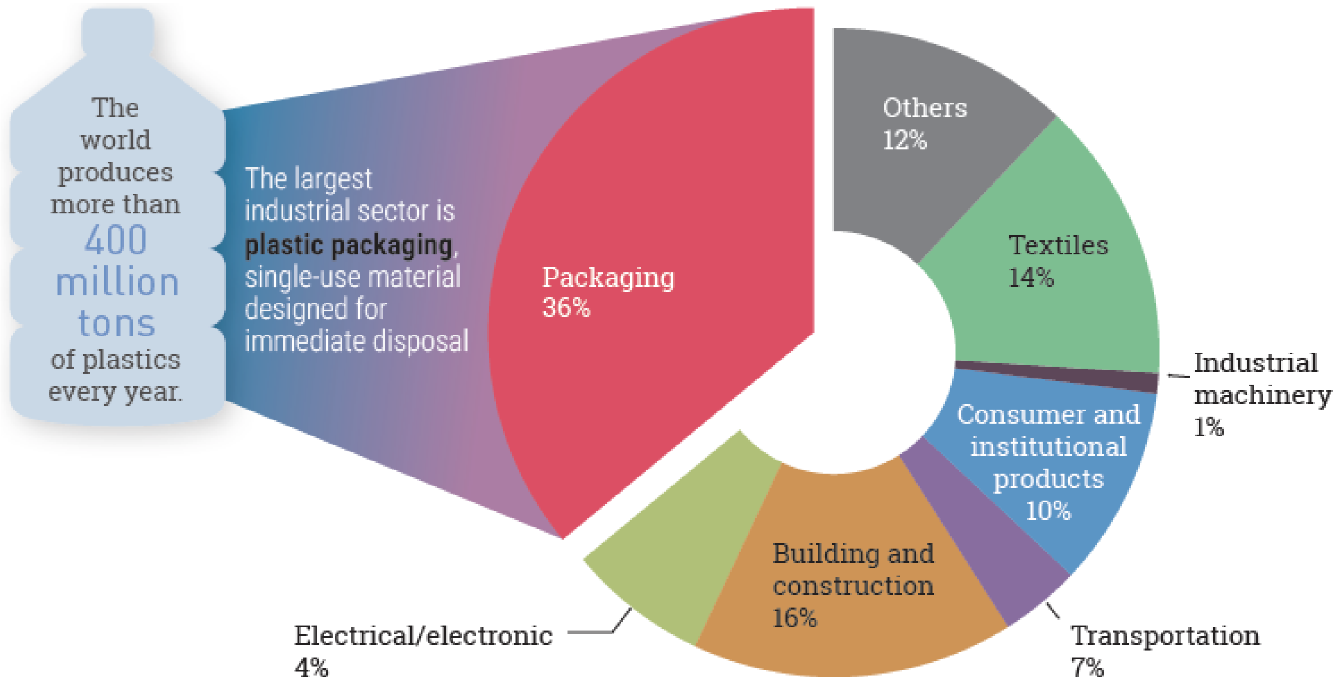
https://committee.iso.org/files/live/sites/tc61/files/
The%20Plastic%20Industry%20Berlin%20Aug%202016%20-%20Copy.pdf

# Global Industrial Use of Plastics

- Packaging is the largest use for plastics but single use:
  - Plastics used in packaging include: LDPE (30%), PET (23%), HDPE (21%), PP (18%), PS (5%), and PVC (2%)




Global Flow of Packaging Waste

40% Landfill
32% Leakage
14% Incinerated
14% Recycled

*Adapted from Geyer, R., et al. Sci. Adv.* **2017**, *3*, e1700782

- If current trends continue, by 2050, the ocean will contain more plastic than fish, by weight

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*UNEP (2018). Single Use Plastic: A Road Map for Sustainability*

# Majority of Plastics (87%) Fall into Categories 1-6
# Recovery Rates for Plastic Recycling in US are Low

| 1 PETE | 2 HDPE | 3 PVC | 4 LDPE | 5 PP | 6 PS | 7 OTHER |
|---|---|---|---|---|---|---|
| Polyethylene Terephthalate | High-Density Polyethylene | Polyvinyl Chloride | Low-Density Polyethylene | Polypropylene | Polystyrene | Other |
| Common products: soda & water bottles; cups, jars, trays, clamshells | Common products: milk jugs, detergent & shampoo bottles, flower pots, grocery bags | Common products: cleaning supply jugs, pool liners, twine, sheeting, automotive product bottles, sheeting | Common products: bread bags, paper towels & tissue overwrap, squeeze bottles, trash bags, six-pack rings | Common products: yogurt tubs, cups, juice bottles, straws, hangers, sand & shipping bags | Common products: to-go containers & flatware, hot cups, razors, CD cases, shipping cushion, cartons, trays | Common types & products: polycarbonate, nylon, ABS, acrylic, PLA; bottles, safety glasses, CDs, headlight lenses |
| Recycled products: clothing, carpet, clamshells, soda & water bottles | Recycled products: detergent bottles, flower pots, crates, pipe, decking | Recycled products: pipe, wall siding, binders, carpet backing, flooring | Recycled products: trash bags, plastic lumber, furniture, shipping envelopes, compost bins | Recycled products: paint cans, speed bumps, auto parts, food containers, hangers, plant pots, razor handles | Recycled products: picture frames, crown molding, rulers, flower pots, hangers, toys, tape dispensers | Recycled products: electronic housings, auto parts, |
| 19.5 % | 10% | 0 % | 5 % | 1 % | 1 % | varies |

https://www.bluelinelabels.com/glossary-of-resins-containers-decorating/

# Motivation for Chemical Upcycling of Polymers

**Upcycling:** the process of selectively converting waste materials into products with greater value as opposed to traditional recycling which typically converts waste into materials for reuse but with reduced properties (downcycling)

- In the US, plastic materials contribute 13% (34.5M tons) to municipal solid wastes in 2015 with less than 10% recycled, approximately 15% combusted for energy recovery, and the remained sent to the landfill (75%)[1]
- Most recycling of plastic wastes typically involves mechanical processes (primary or secondary recycling: sort, grind, wash, extrude) and is only applied to limited plastic types but the products are cheaper than new materials
- More energy is saved by recycling than recovered by burning plastic (heating value of plastics 36 MJ $kg^{-1}$ while mechanical recycling conserves 60 – 90 MJ $kg^{-1}$)
- On average, each tonne of plastic recycled saves the energy equivalent in the combustion of 22 barrels of oil[2]
- Increased plastic recycling is an important pathway to reduce plastic waste and has clear energy, economic, and environmental impacts
- Opportunity exists for fundamental research to provide the foundational knowledge needed to design chemical reactions, processes, and materials that enable efficient, low-temperature conversion of discarded plastics to high-value chemicals or materials



[1] *Advancing Sustainable Materials Management: 2015 Fact Sheet*; EPA530-F-18-004; UE EPA : Washington, DC, July, 2018.

[2] Rahimi, A.; García, J. M. *Nat. Rev. Chem.* **2017**, *1, Article Number* 0046

# Challenges for Chemical Upcycling of Polymers

- Difficult to sorting plastics to get a clean stream (density, electrostatics, wettability, spectral signature)
- Plastics are not pure and contain additives, food residues, dirt, degradation products, etc. that could impact upcycling
- Polyolefins are often combined with other materials in multi-layer packaging which can not be recycled
- High chemical, thermal, and mechanical stability of polymers provide challenges to deconstruction (and thus, new chemistry is needed)
- Thermosets are crosslinked polymers that can not currently be recycled by mechanical, thermal, or solvent processing methods

| **Additives in Polymers** | **Percentage** |
|---|---|
| Plasticizers | 34% |
| Flame retardants | 13% |
| Heat stabilizers | 5% |
| Fillers | 28% |
| Impact modifiers | 5% |
| Antioxidants | 6% |
| Colorants | 2% |
| Lubricants | 2% |
| Light stabilizers | 1% |
| Other | 4% |

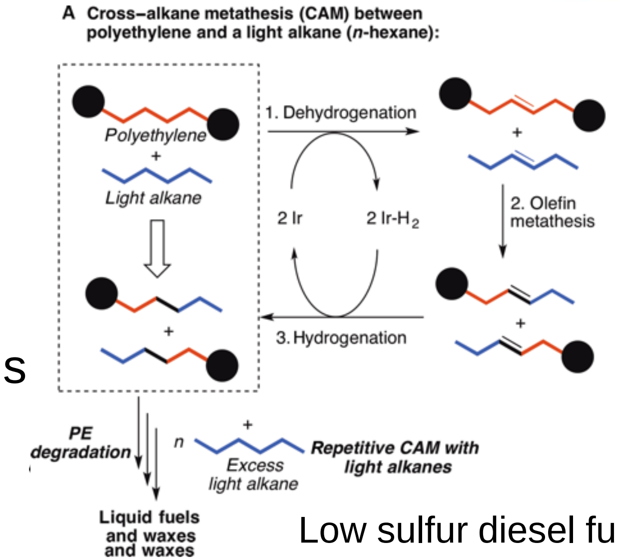
*Geyer, R. et al., Sci. Adv.* **2017**, *3,* e1700782

# The World is Reevaluating the Plastic Economy

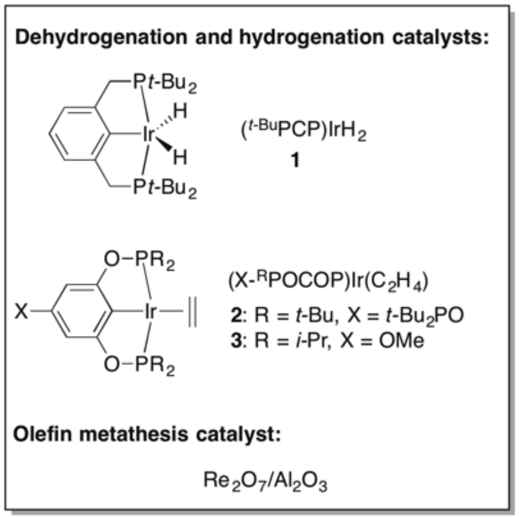
- In 2016, two reports published by World Economic Forum, the Ellen MacArthur Foundation and McKinsey & Company which makes the case for rethinking the current plastics economy and identifies a number of significant knowledge gaps and open questions
  - *The New Plastics Economy – Rethinking the future of plastics*
  - *The New Plastics Economy – Catalyzing Action*
- In the second report, three distinct strategies were proposed to accelerate the shift towards the new plastics economy

# Energy Efficient Chemical Upcycling of Polymers Aligns with DOE BES Mission

- Fundamental chemical and materials sciences required to enable upcycling of polymers fall directly within BES's and DOE's energy mission
- BES research has contributed significantly to the scientific foundations in catalysis, thermochemical kinetics, control of chemical transformations, materials synthesis (control of structure and properties) and characterization, biosciences (bio-inspired catalysts), and computational modeling required to advance a fundamental research agenda in polymer construction, deconstruction and reassembly
- Strength in understanding the link between atomic and molecular scale organization and bulk properties
- Unique strength in combining research in chemical and natural systems
- Unique tools (neutrons, x-rays, nanoscience, and computation) to support atomic scale and mesoscale research in upcycling




Low sulfur diesel fuel



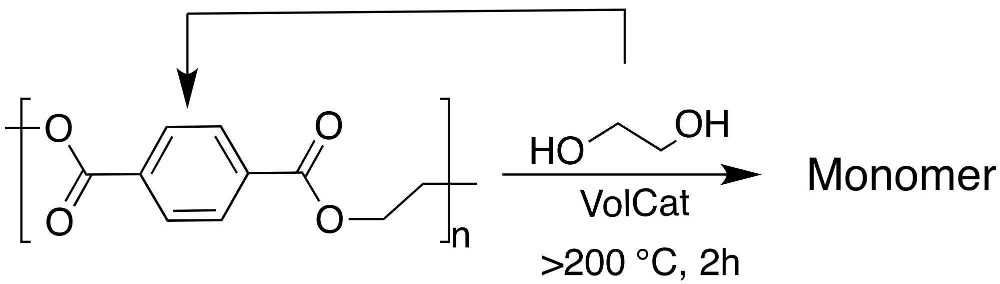

Jia, X. et al. *Sci. Adv.* **2016**, *2*, e1501591

# Opportunities in Chemical Upcycling of Polymers

- This Roundtable will focus on four challenges and research opportunities for chemical upcycling of polymers that build off the strengths in BES portfolio
  - Design chemical mechanisms to deconstruct polymers and create targeted molecular intermediates that provide building blocks for new products
  - Create integrated depolymerization-reassembly processes that target high-value end products from starting polymers
  - Design next-generation polymeric materials that enable efficient depolymerization-reassembly
  - Investigate crosscut opportunities for advancing experimental, computational and data science driven approaches for upcycling of polymers

# Challenge 1:
# Design Chemical Mechanisms for Deconstruction

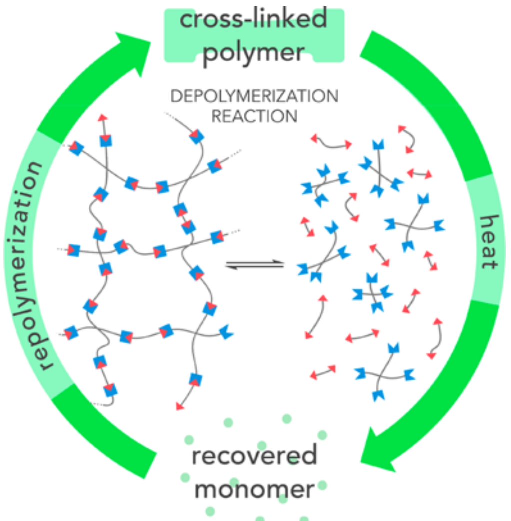
- Design chemical mechanisms to deconstruct polymers and create targeted molecular intermediates that provide building blocks for new products
  - For example, IBM has developed a process that separates contaminants (e.g., food residue, glue, dirt, dyes, and pigments) from PET and produces pure monomer in an energy-efficient cycle



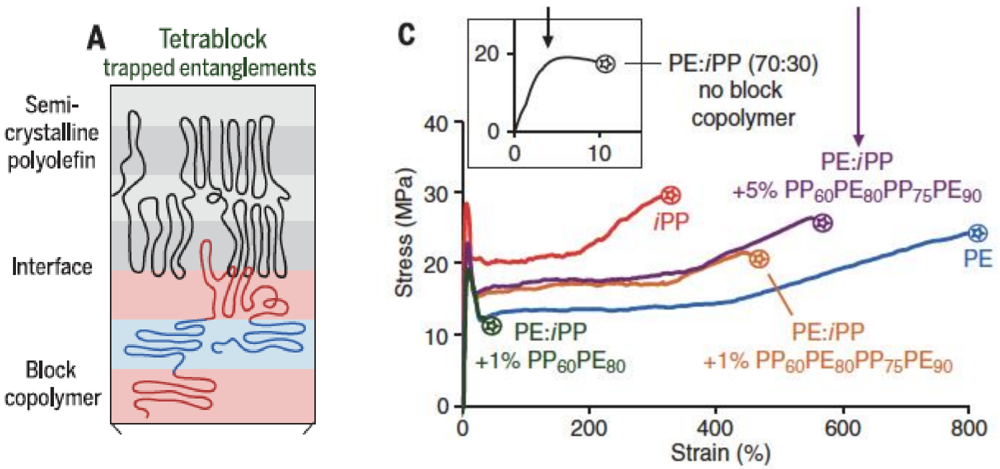

https://www.research.ibm.com/5-in-5/trash/

# Challenge 2:
# Create Integrated Deconstruction-Reassembly Processes

- Create integrated depolymerization-reassembly processes that target high-value end products from starting polymers
  - For example, most processes today take polymers back to monomers and then repolymerize to products with similar performance
  - Another approach is to process immiscible polymers, such as polyethylene and isotactic polypropylene, by stitching together with a block copolymer



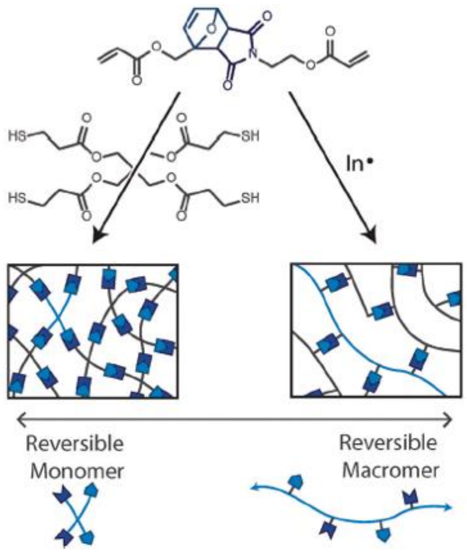

Fortman, D. J. et al. *ACS Sustainable Chem. Eng.* **2018**, *6*, 11145



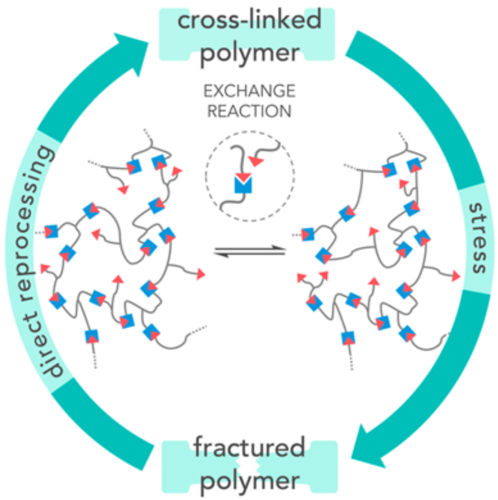

Eagan, J. M. et al. *Science* **2017**, *355*, 814

# Challenge 3:
# Design Next Generation Recyclable Polymers

- Design next-generation polymeric materials that enable efficient depolymerization-reassembly
  - Significant interest in recycling thermosets (cross-linked polymers) which are 15-20% of the market but currently are not recyclable or reprocessable
  - Examples of approaches to depolymerization and reprocessing thermosets include:
    - Dynamic covalent networks and covalent adaptive networks (CAN)
    - Vitrimers – a strategy for direct mechanical reprocessing where polymers rearrange their topology by exchange reactions without depolymerization




Kloxin, C. J. et al., *Chem. Soc. Rev.* **2013**, *42*, 7161




Fortman, D. J. et al. *ACS Sustainable Chem. Eng.* **2018**, *6*, 11145

# Goal: Chemical Upcycling of Polymers Roundtable

- Convene a small group (ca. 20) of experts from industry, academia, and national labs to address fundamental challenges to enable transformation of discarded plastics to high-value fuels, chemicals, and materials
- Prepare a factual document to provide the workshop participants with a high-level assessment of the current status of polymer upcycling
- Identify priority research opportunities in which fundamental research over the next 5-10 years could result in a significant impact on chemical upcycling of polymers
- Prepare a report which captures these possible priority research opportunities for chemical upcycling of polymers
- **Status:**
  - Chairs confirmed; Panel Leads selected/contacting; Participants almost final
  - Date, Location selected: April 30 – May 1; Bethesda North Marriott
  - Factual Document being written (completed draft delivered mid-April)
  - Webinar in advance of the workshop (tentatively mid-late April)

# Polymer Upcycling Roundtable - Format

- Introductory remarks by DOE-SC leadership
- Goals and logistics
- Presentations: Three short presentations on polymer upcycling
- Panel discussion on each focus area (with cross-cut integrated):
  - Each participant will come prepared to discuss roadblocks, knowledge gaps, research needs, and research opportunities
    - Mechanisms for deconstructing to molecular intermediates
    - Create integrated deconstruction-reassembly processes
    - Design next generation recyclable polymers
- Report out
- Refine Priority Research Opportunities (PRO)
- Final report out of Priority Research Opportunities
- Report writing - writers and panel leads stay extra half day to capture input and pull together a rough draft

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  - Design chemical mechanisms to deconstruct polymers and create targeted molecular intermediates that provide building blocks for new products
  - Create integrated depolymerization-reassembly processes that target high-value end products from starting polymers
  - Design next-generation polymeric materials that enable efficient depolymerization-reassembly
  - Investigate crosscut opportunities for advancing experimental, computational and data science approaches for chemical upcycling of polymers