Center for Plastics Innovation (CPI) EFRC Director: LaShanda Korley Lead Institution: University of Delaware Class: 2020 – 2024

Mission Statement: To develop catalytic and functionalization approaches and fundamental tools applicable to the upcycling of polymer plastics waste, with a strategic focus on enabling mixed-stream transformations from varied material form factors

We will develop a comprehensive polymer plastics waste (PPW) upcycling strategy that combines fundamental discoveries in catalytic technology and chemical functionalization with innovations in polymer design and additive manufacturing and is enabled by the leveraging of computational, data science, characterization, and systems design tools. We will target these scientific pursuits toward the transformation of complex PPW streams into high-value fuels, lubricants, monomers, and functional polymers. Specific to our approach is the integration of multiscale considerations of evolving materials complexity during upcycling, predictive strategies to accelerate discovery, and less energy-intensive



processing considerations. These objectives will nucleate a transition from the current high-energy and lower-value landscape of polymer recycling to a new frontier of polymer upcycling strategies that utilize low-temperature and selective catalytic and engineering approaches to obtain high-value and functional materials.

Description: We will leverage our expertise in catalysis (synthetic, biological), macromolecular science and engineering, additive manufacturing, data science and artificial intelligence (AI), systems engineering, and computation to address three distinct thrusts: (1) tunable heterogeneous catalysts and microwave (MW) energy for the conversion of PPW into fuels, lubricants, precision macromolecules, and monomers,

(2) functionalization and upcycling using *a*) plasma-assisted, catalysis and surface treatment, *b*) photoredox-catalyzed decarboxylation, and *c*) enzymatic routes to generate high-value monomers and polymers, and (3) new cross-cutting tools driven by AI, macromolecular characterization, and additive manufacturing to enable scientific advances. *CPI* will overcome distinct challenges related to PPW upcycling, including *PPW diversity and heterogeneity; optimization of macromolecule/catalyst interactions in melt; selectivity control;* and *development of correlations between plastics manufacturing, chemical recycling, and macromolecular physical properties.*

Methods: We will fabricate *hierarchical, multiscale materials* to study interactions between complex PPW and multifunctional catalysts, employ *real-life PPW* to validate our fundamental studies, utilize *bioenzymatic* and *chemical transformations* to add value to polymers waste, design *energy-efficient MW technology* and innovative *plasma-functionalization* strategies, develop *multiscale modeling* and *data mining* tools to enhance predictive capabilities, target *system-level* approaches, harness *new polymer chemistry* and *manufacturing* techniques for valorization, and develop advanced *spectroscopic techniques* for complex media – all to form a basis for significant advances in PPW upcycling.

Impact: We will transform the current high-energy/low-value landscape of polymer recycling towards highly efficient polymer upcycling strategies. Mechanistic insights in MW-assisted, low-temperature catalysis for depolymerization in the melt, plasma-assisted functionalization approaches, photoredox decarboxylation strategies, and enzyme engineering to valorize PPW will provide immense fundamental knowledge. Cross-cutting tools and processes will impart long-lasting impact on science and technology. Furthermore, our systems-level approach will tackle real-life PPW to define new frontiers in research and educational training with direct impact on polymer upcycling, chemistry, manufacturing, catalysis, and data science.

Overarching Goals and Objectives: The complexity of converting PPW presents numerous opportunities for scientific discovery and technological innovation in catalysis, polymers, materials, modeling, and AI science. We will develop a comprehensive program with the **overarching goal** to overcome the fundamental knowledge barriers described above toward advancing PPW chemical recycling and upcycling strategies. *CPI* will focus on PPW spanning from single-stream to multi-component products containing PET, HDPE, LDPE, PP, PS, and PMMA. It will lay the foundation for fundamental science to allow the design of fuels, lubricants, monomers, and macromolecules, as well as enable upcycling with targeted functionality to new polymer structures. The **objectives of** *CPI* include: (1) develop approaches and fundamental tools applicable to the upcycling of real PPW, with a strategic focus on enabling mixed-stream transformations in varied material form factors (*i.e.*, solutions, melts, and surfaces); (2) educate the future U.S. workforce for relevant industries; and (3) enable PPW upcycling innovations *via* technology transfer, licensing, and start-up formation.

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