Emerging Frontiers in Research & Innovation (EFRI)

FY21 Solicitation: NSF 20-614

EMERGING FRONTIERS & MULTIDISCIPLINARY ACTIVITIES (EFMA)

OFFICE HOUR NOVEMBER 9TH, 2020

Office Hour Agenda

1. Welcome and Introductions
2. Overview of EFRI
3. Topic 1: Distributed Chemical Manufacturing – DCheM
4. Topic 2: Engineering the Elimination of End-of-Life Plastics – E3P
5. Q & A

EFRI Team Members

EFMA Office

- Sohi Rastegar, Head
- Louise R. Howe, Program Director
- Alias J. Smith, Associate Program Director
- Garie Fordyce, Expert
- Tammy Wilbert, AAAS STPF Fellow
- Terria Davis, Program Specialist

EFRI Program Directors

DCheM: Distributed Chemical Manufacturing	E3P: Engineering the Elimination of End-of-Life Plastics
Topic Coordinator: Raymond Adomaitis – ENG/CBET	**Topic Coordinator:** Christina Payne – ENG/CBET
Carole Read – ENG/CBET	Bruce Hamilton – ENG/CBET
Robert McCabe – ENG/CBET	Catherine Walker – ENG/CBET
William Olbricht – ENG/CBET	Steven Peretti – ENG/CBET
Karl Rockne – ENG/CBET	Khershed Cooper – ENG/CMMI
Ying Sun– ENG/CBET	David Rockliffe – BIO/MCB
Thomas Kuech– ENG/CMMI	Suk-Wah Tam-Chang – MPS/CHE

Key website

Office of Emerging Frontiers & Multidisciplinary Activities (EFMA) Website:

http://www.nsf.gov/eng/efma

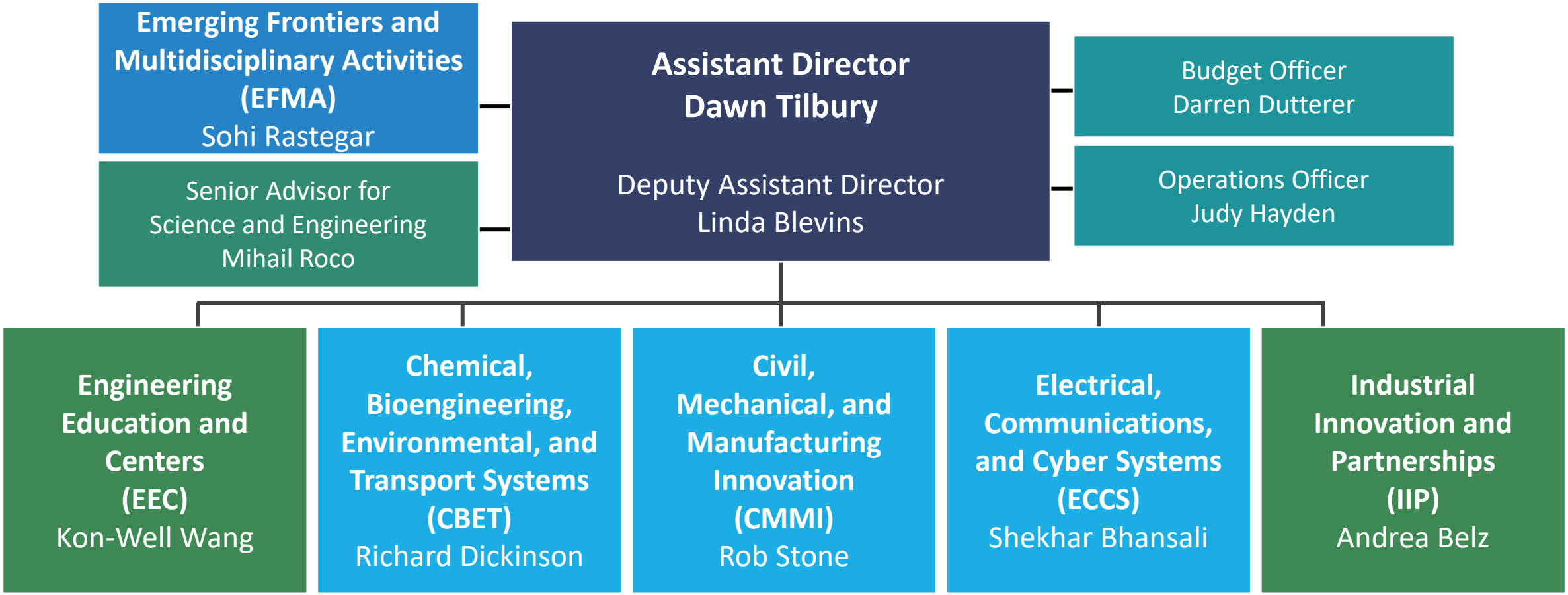
Please refer to this website for up-to-date information.

Goals of Office Hour

- To inform the community about the EFRI FY 2021 Program Solicitation.

- To respond to questions from potential applicants.

NSF Directorate for Engineering



Emerging Frontiers in Research and Innovation (EFRI)

$2m awards

15-16 awards/year

Supports high-risk, high-reward opportunities that:

- Are potentially transformative
- Address a national need or grand challenge
- Involve multi- or inter-disciplinary research
- Have a leadership role for Engineering

EFRI FY21 Topics
(Solicitation NSF 20-614)

- **DCheM**: Distributed Chemical Manufacturing
- **E3P**: Engineering the Elimination of End-of-Life Plastics

EFRI FY21: Key Solicitation Information

Due Dates

- **Letter of Intent (*required*): December 9, 2020**
- **Preliminary Proposal (*required*): January 5, 2021**
- **Full Proposal: April 19, 2021**

Team proposals Only: 3-5 PIs/co-PIs

Awards are up to 4 years and up to $2M over grant lifetime

Limit on Number Proposals per Individual (PI or co-PI): One per Topic

Proposals may be submitted by a single organization or group of organizations

2021 EFRI DCheM Overview

NSF 20-614

Ray Adomaitis (radomait@nsf.gov)
Program Director
Process Systems, Reaction Engineering, and Molecular Thermodynamics
9 November 2020

DCheM overview

Distributed Chemical Manufacturing aims to revolutionize the chemical process industries by enabling intensified and, where appropriate, modular process plants, that take advantage of distributed resources and/or address distributed environmental remediation needs.

The *unifying theme of DCheM-inspired research* is to merge expertise on chemical and physical phenomena at the molecular, cellular and process scales with models at multiple scales (from quantum mechanical and atomistic to process and enterprise levels), advanced process control/optimization methods, and data science algorithms to develop novel processes that are compact, efficient and environmentally friendly.

DCheM thrusts

1. Fundamental chemical and physical transformation of matter, including reaction kinetics and transport phenomena, alternative means of reaction activation
2. Process integration and advanced manufacturing, including multifunctional process units and microchemical systems
3. Process modeling, optimization, and control, including multiscale and reduced-order modeling, machine learning, real-time optimization

New for FY21: Thrust 1 is required and thrusts 2 and/or 3 must be addressed

D is for Distributed

New for FY21:

Preliminary and full proposals must provide a compelling argument for need for/benefits of being geographically distributed. Evidence must be given that traditional process economic, energy use, and other sustainability scaling relationships do not apply. Estimates of the life cycle energy use and/or greenhouse gases and regulated emissions impacts are highly encouraged for the distributed manufacture method versus the predominate status quo method and state-of-the-art in the literature.

EFRI solicitation-specific criteria

- **TRANSFORMATIVE -** Does the proposed research present an opportunity for a significant leap or paradigm shift in fundamental engineering knowledge?
- **NATIONAL NEED/GRAND CHALLENGE -** Is there potential for making significant progress on a national need or grand challenge?
- **BROADENING PARTICIPATION PLAN -** Does the plan actively promote, increase, and enhance the participation of underrepresented groups in the field of engineering and in engineering research?

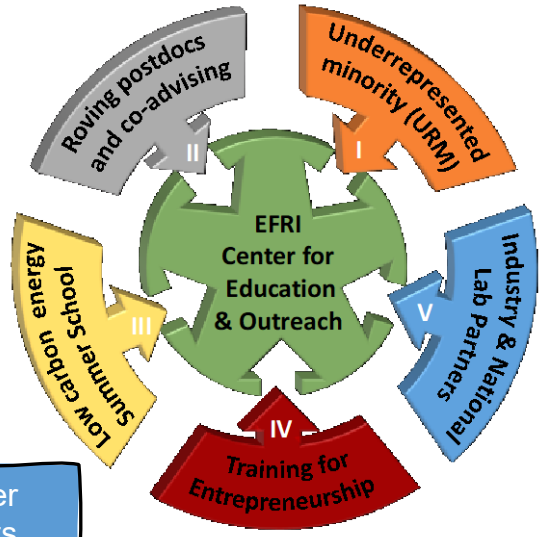
Engineering interfaces between plasma, catalysts, and reactor design for natural gas conversion to liquid products 2029425

Princeton University
Prof. Michele L. Sarazen (PI)
Prof. Yiguang Ju (Co-PI)

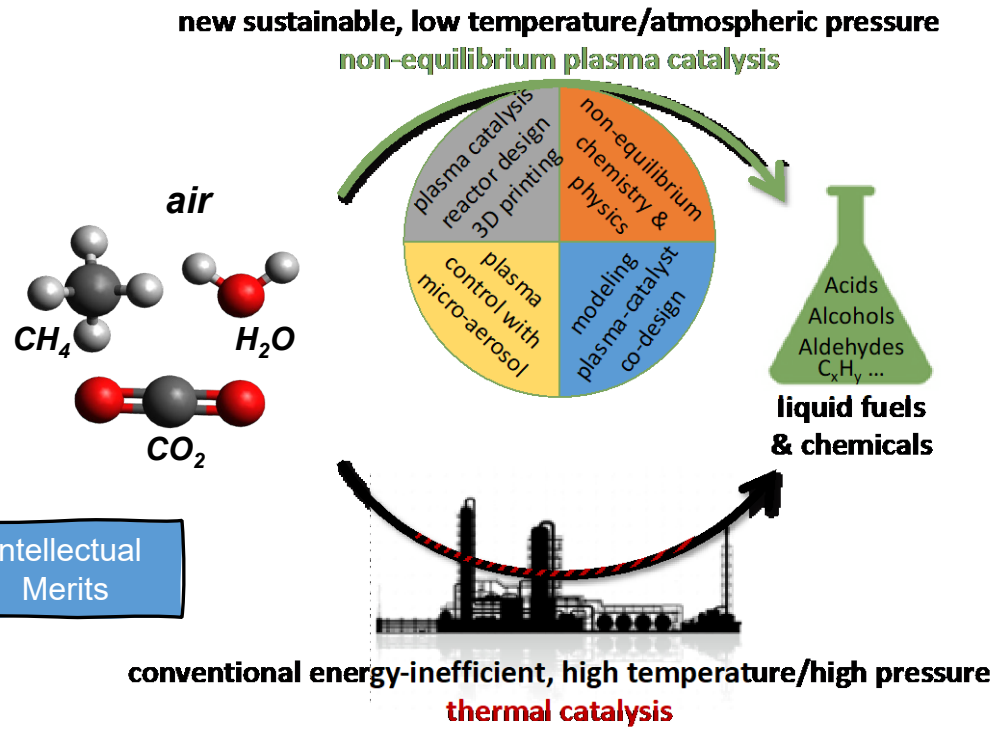
University of South Carolina
Prof. Lang Yuan (Co-PI)
Prof. Tanvir Farouk (Co-PI)
Prof. Sang Hee Won (Senior Personnel)

Stanford University
Prof. Xiaolin Zheng (Co-PI)

Broader Impacts



Intellectual Merits



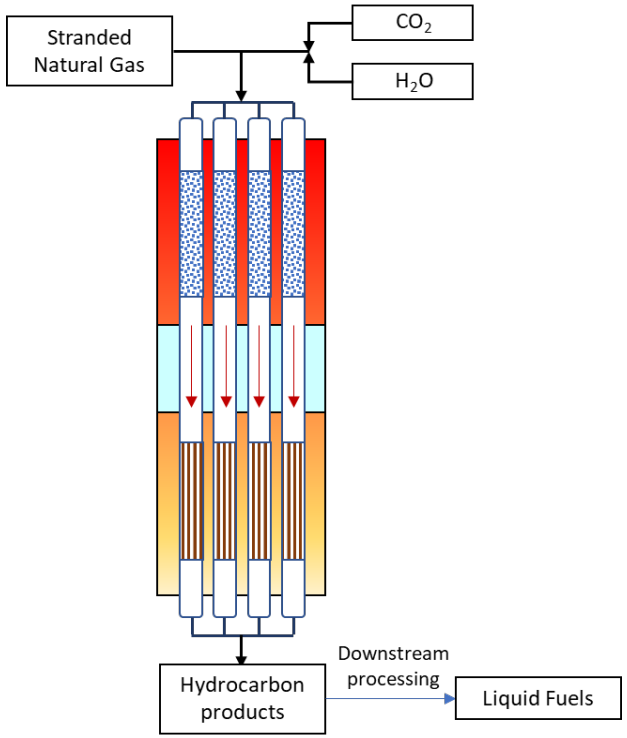
Engineering and enhancing interfaces through…

- design of plasma catalysts and characterization of plasma catalysis reaction pathways
- hybrid plasma generation, and its control of stability and reactivity, in atmospheric multiphase (micro aerosol) plasma reactors
- advanced diagnostics tools for non-equilibrium plasma catalysis processes in the chemical and physical transformation of matters
- innovative design and catalyst integration of distributed **M**icro-**A**erosol **P**lasma **C**atalysis **R**eactor (**MAPCAR**) via additive manufacturing
- optimization via experimentally validated multiscale modeling tools for plasma, chemistry, and reactor design
- academic, national lab, and industrial partnerships

One-step conversion of CH_4 and CO_2 to liquid fuels with the use of a multi-functional pseudo catalytic system

2029282

PI: Dr. Liang-Shih **Fan**, The Ohio State University
Co-PI: Dr. Vicky Doan-Nguyen, The Ohio State University
Co-PI: Dr. Andrew Tong, The Ohio State University
Co-PI: Dr. Joel Paulson, The Ohio State University
Senior Personnel: Dr. Heinz Robota, Velocys Inc.
Senior Personnel: Dr. Jan Lerou, Jan Lerou Consulting, LLC

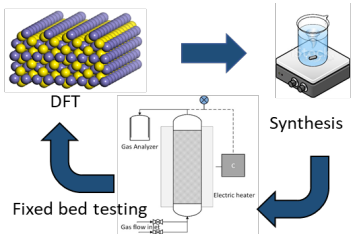


Overall Reaction:

$$CH_4 + CO_2 + H_2O \rightarrow C_5^+\ HC\ products\ (Liq.Fuel)$$

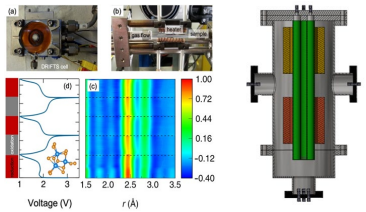
Objective: **Enable advanced spatiotemporal process intensification by designing a cost-effective metal-oxide based modular reactor system for stranded gas valorization**

Year 1



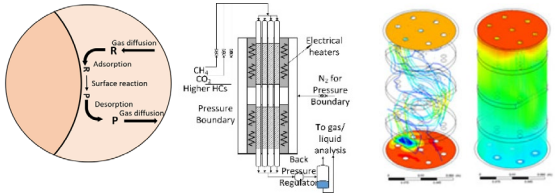
Advanced materials development for improved catalytic activity

Year 2



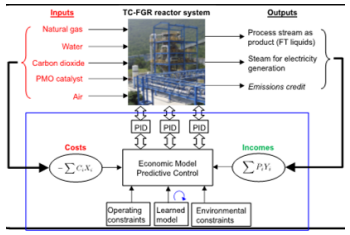
Reaction modelling & bench scale reactor design and optimization

Year 3



Bench-scale reactor fabrication and integration of reactor model for a commercial system

Year 4



Commercial design, techno-economics and advanced control strategies development

Additional FY20 awards

Distributed Manufacturing of Personalized Medicines
2029139; PI: Max Shtein; Co-PIs: Nair Rodriguez-Hornedo, Ronald Larson, Anish Tuteja, Geeta Mehta; University of Michigan

Modular SynBio Processing Units for Distributed Manufacturing of High-Value Products
2029249; PI: Lilo Pozzo; Co-PIs: Hal Alper, James Carothers, Alshakim Nelson, Nadya Peek; University of Washington

Renewable Energy Driven Electrocatalytic Co-Conversion of CO2 and Regional Feedstocks to Chemicals and Fuels
2029326; PI: David Flaherty; Co-PIs: Andrew Gewirth, Paul Kenis, Joaquin Rodriguez Lopez, Ashlynn Stillwell; University of Illinois at Urbana-Champaign

Additional FY20 awards

Next-generation Low Global Warming Refrigerants
2029354; PI: Mark Shiflett; Co-PIs: Edward Castner, Edward Maginn, Emily Pentzer; University of Kansas

Precise but Tunable Reactions Through Tunably Precise Surfaces
2029359; PI: William Epling; Co-PIs: Lars Grabow, Andrew Teixeira; University of Virginia

Electrifying CO2 From Point Sources into Pure Liquid Fuels
2029442; PI: Haotian Wang; Co-PIs: T. Alan Hatton, Rafael Verduzco, Yuanyue Liu; William Marsh Rice University

TOPIC 2: Engineering the Elimination of End-of-Life Plastics (E3P)

Goal: Establish requisite knowledge and methods to enable technologies that depolymerize and recapture value from end-of-life plastic materials

- Chemical and/or biological depolymerization and valorization
- Novel methods and processes associated with plastic manufacturing and recycling frameworks

Engineering the Elimination of End-of-Life Plastics (E3P)

To achieve effective management of end-of-life plastic waste...

Robust physical systems and materials for plastic lifecycle management, including sensors for detection and characterization of composition and reaction dynamics, and mass separating agents for capture of plastic materials and plastic-derived molecules;

Development of novel catalysts and reaction engineering, either chemical or biological, enabling complete depolymerization and/or valorization of plastic waste; and

Systems-level integration of new plastic remediation and valorization technologies into manufacturing infrastructures, including improving efficiency and economic viability of existing recycling, remediation, and valorization technologies.

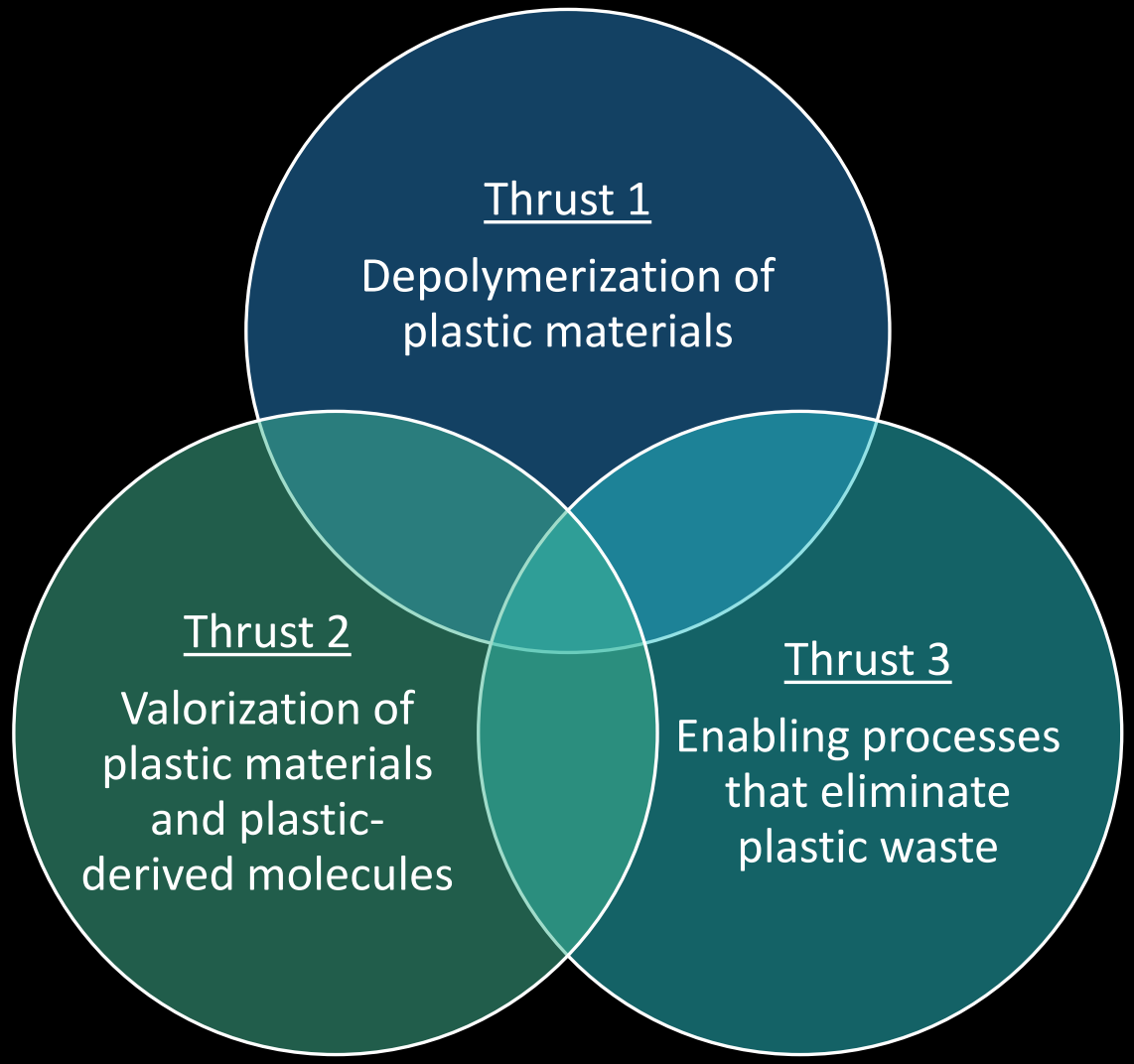
Engineering the Elimination of End-of-Life Plastics (E3P)

EFRI 2021 E3P Team Members

Christina Payne (ENG/CBET) – E3P Topic Coordinator

- Bruce Hamilton, ENG/CBET
- Catherine Walker, ENG/CBET
- Steven Peretti, ENG/CBET
- Khershed Cooper, ENG/CMMI
- David Rockcliffe, BIO/MCB
- Suk-Wah Tam-Chang, MPS/CHE

E3P: Research Thrusts



Thrust 1: Depolymerization of plastic materials

Goal: Engender transformative approaches capable of depolymerizing plastics into molecular components for future use or environmentally benign disposal

- Simultaneous targeting of several polymer types is encouraged

Chemical depolymerization

- Robust catalysts capable of selective bond activation/functionalization or improved reaction rates
- Chemical reaction engineering, including reactor designs for processing polymers and deploying heterogeneous catalysts
- Understanding of complex reaction networks and mechanisms, macromolecular thermodynamics, and transport properties

Biological depolymerization

- Tailored microbial system design
- Protein engineering

Thrust 2: Valorization of plastic materials and plastic-derived molecules

Goal: Develop pathways and systems for plastics and depolymerization products to re-enter the value chain, incentivizing collection and recycling of plastic waste

- Formulation of new chemical, biological, and/or physical valorization processes and understanding of the attendant mechanisms
- Closely coupled with depolymerization processes, high-value fuels and chemical products, easily separable intermediates
- Theories, models, and tools for design and prediction of new routes to polymeric products and monomers
- Reaction design for polymer-to-polymer synthesis
- Combining modeling and experiments to understand and control molecular processes
- Reactive polymer processing methods, advanced manufacturing systems, and systems-level integration

Thrust 3: Enabling processes that eliminate plastic waste

Goal: Promote development of innovative materials, methods, tools, and physical systems that complement processes for the elimination of end-of-life materials and valorization of polymeric products

Separation of plastics and plastic-derived molecules from chemical process streams and water sources

- Mass separating agents for selective removal of products/monomers
- Low-energy solvent- or electrochemical-based separations
- Membranes for separation of micro- and nano-plastics from water and process effluent

Real-time detection of chemical properties and reaction dynamics, broadly defined

- High-throughput analytical techniques for characterization of municipal mixed waste streams
- Real-time, in situ reaction monitoring and control

E3P Requirements

- Interdisciplinary team
- At least one engineering investigator
- Inclusion of a physical or biological scientist is strongly encouraged
- Research plan must address **at least two of the three thrusts**
- PIs must consider the ethical, social, economic, health, legal, and environmental implications of their proposed research, and discuss these as appropriate
- Substantial collaborations with ethicists, environmental scientists, behavioral scientists, and/or economists are encouraged, if applicable.