Linda Sapochak, Division Director
Division of Materials Research

MPS Representative for ERE WG

**Directorate for Mathematical & Physical Sciences (MPS):**

*Accelerating Research and Innovation on a Changing Planet*

ERE-AC meeting, November 3-4, 2021
CHE - Environmental Chemical Sciences (ECS)

......supports experimental and computational research on the fundamental chemistry of processes in the environment. Recognizing the intrinsic complexity and heterogeneity of environmental systems, projects develop and utilize advanced experimental, modeling and simulation approaches to discover, explain, and predict environmental phenomena at the molecular scale. Topics may include, but are not limited to: processes occurring at environmental interfaces and the chemical behavior and transformation under a variety of naturally occurring environmental conditions.

EAGER: CAS-MNP: Effect of Sunlight on Fate and Transport of Nanoplastics and Associated Organic Pollutants in Aquatic Systems, Matthew A. Tarr (PI), Phoebe A. Zito (co-PI), University of New Orleans
Division of Chemistry

- Division of Chemistry: Disciplinary Research Programs (CHE-DRP)
- Chemical Catalysis (CAT)
- Chemical Measurement and Imaging (CMI)
- Chemical Structure, Dynamics, and Mechanisms A (CSDM-A)
- Chemical Structure, Dynamics, and Mechanisms B (CSDM-B)
- Chemical Synthesis (SYN)
- Chemical Theory, Models, and Computational Methods (CTMC)
- Chemistry of Life Processes (CLP)
- Environmental Chemical Sciences (ECS)
- Macromolecular, Supramolecular, and Nanochemistry (MSN)

Division of Materials Research

- Division of Materials Research: Topical Materials Research Programs (DMR-TMRP)
- Biomaterials (BMAT)
- Ceramics (CER)
- Condensed Matter and Materials Theory (CMMT)
- Condensed Matter Physics (CMP)
- Electronic and Photonic Materials (EPM)
- Metals and Metallic Nanostructures (MMN)
- Polymers (POL)
- Solid State and Materials Chemistry (SSMC)

Credit: Michaela Burke
MPS Core Programs Support Climate Mitigation Research

DMR-POL: Design of Inherently Recyclable Plastics

*Synthesis of a Vitrimer and Its Network Structure*

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\begin{align*}
\text{PE-OTMS network}
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Macroscopic Polymer (Re)Processing

CHE-CAT: Transforming carbon waste streams

Discovering new catalysts to transform CO₂ waste streams into useful chemicals.

Hialiang Wang’s group at Yale developed a molecular electrocatalyst that converts CO₂ into methanol.


PI: Zhibin Guan (University of California, Irvine)
The CAS Program seeks to support basic research through core disciplinary programs aimed at improving the sustainability of resources for future generations while maintaining or improving current products to offer technologically-advanced, economically competitive, environmentally-benign and useful chemicals & materials to a global society.

To address these challenges, the program aims to identify opportunities for innovation in a wide range of contributing disciplines as well as integrative activities. This program encourages the development of new experimental and theoretical/modeling approaches that will aid in both reductionist and whole-systems approaches.
Critical Aspects of Sustainability (CAS) - DCLs

• Dear Colleague Letter: **Critical Aspects of Sustainability (CAS): Micro- and Nanoplastics (MNP)** – MPS (CHE, DMR), ENG (CBET, CMMI), GEO (EAR, OPP), BIO (DEB), EHR (DRL, DUE), OD (OISE)

• Dear Colleague Letter: **Critical Aspects of Sustainability (CAS): Innovative Solutions to Climate Change** – MPS (CHE, DMR, DMS, PHY), ENG (CBET, CMMI, ECCS, EEC, IIP) GEO (AGS, EAR, OCE), BIO (DEB, IOS, MCB), CISE (CCF, CNS, OAC, IIS), EHR (DGE, DRL, DUE, HRD), SBE (BCS, SES) and OD (OISE)
Objectives:
• This project combines experimental and computational approaches to understand how environmental weathering by sunlight or microorganisms affect the adsorption of organic contaminants on microplastics.
• The data will be utilized to train statistical predictive models.
Focusing on solutions: *Mitigation* and Adaptation

1. Reduction of GHG emissions and energy use
2. Energy innovations
3. GHG Sequestration and Removal
4. Climate Change Adaptation
5. Synergistic Topics

* Mitigation: efforts to reduce the amount and speed of future climate change by limiting emissions or removing carbon dioxide from the atmosphere
https://www.globalchange.gov/

The Physics Division is a lead participant in the ECLIPSE metaprogram that has been created to foster an ecosystem spanning multiple NSF Directorates in the pursuit of translational research at the interface of fundamental plasma science and technological innovation.

In the environmental area these include atmospheric pressure plasmas and microplasmas with applications to, e.g., microelectronics, plasma medicine, plasma agriculture, environmental remediation, and other clean energy goals enabled by electrification of the chemical industry.
MPS Team & Center Programs

Next competition starts Fall 2022
• By embedding an industrially relevant catalyst, it was demonstrated that post-consumer polyurethane foam can be remolded into rubber or plastic using twin-screw extrusion at elevated temperatures.

• It was shown that the resulting recycled material maintains its mechanical properties after the process is complete. Additionally, air present in the initial foam waste is removed during the screw mixing process which produces rubber or plastic.

• Because this process was demonstrated on commercially sold material, this method has the potential to enable the recycling of the vast amounts of polyurethane foam waste into rubber or plastic products.


**Focus:**
Scalable production of bio-derived building blocks and polymers from yeast, fungi and bacteria. Data-driven discovery of next-generation polymers with properties and performance far exceeding those currently available in materials produced through traditional petrochemical-based methods.

**Major User Facilities:**
- Living Bioreactor: automated gene assembly, amplification, transformation, strain growth, and metabolite analysis.
- Synthetic Chemistry: robotic synthesis, flow chemistry, and 3D printing.
- Characterization: Next-generation XRD, microRheology; microED.
- Data and Computation: multiscale biopolymer simulation.

www.biopacificmip.org
MPS User Facilities

- National High Magnetic Field Laboratory (NHMFL)
- Center for High-Energy Synchrotron Science (CHEXS) at CHESS/Cornell
- Center for High Resolution Neutron Scattering (CHRNS) at NIST
- ChemMatCARS – Applied Photon Source, Argonne Nat. Lab./Univ of Chicago
- National Nanotechnology Coordinated Infrastructure (ENG, MPS)
- Materials Innovation Platforms (MIPs)
- The Daniel K. Inouye Solar Telescope, located on Haleakala on the Island of Maui, Hawaii
Mission

- Operate a world-leading high-magnetic-field user program
- Carry out in-house research in support of the user program
- Maintain facility and develop new magnets/instrumentation
- Conduct education and outreach activities

DC Field

Pulsed Field

ICR

45 T hybrid magnet

101 T pulsed fields

21 T / 123 mm ICR

NMR

EMR

AMRIS

HBT

21.1 T / 105 mm NMR

W-Band HiPER Spectrometer

11 T / 400 mm MRI

<1 mK High B/T

DMR & CHE
14 T high-homogeneity wide-bore magnet, 100 part-per-billion mass resolution

petroleum and metabolic compounds

More than 100,000 different molecules in oil and different for each oil well

Mass in Dalton (a.m.u.)

Improved Resolution with FT-ICR

QqTOF (the primary competing technique)

C_{8}H_{9}N_{3}O_{2}^{+} m/z 178.06110

C_{7}H_{8}N_{5}O^{+} m/z 178.07234

C_{12}^{13}C_{1}H_{9}N_{4}O^{+} m/z 178.08044

C_{8}H_{10}N_{4}O^{++} m/z 178.08491
**What is the finding?** In a matter of weeks, sunlight can chemically transform marine plastics into thousands of compounds that dissolve in the ocean. The number and characteristics of these compounds differ between consumer plastic shopping bags (from Target, CVS, and Walmart) and pure polyethylene, the polymer used to make these bags. These differences are driven by chemicals added to the plastics to improve performance and appearance, as well as to lower costs.

**Why is this important?** Plastic was initially believed to be inert in the environment. This work contributes quantitative information to the growing understanding that sunlight can transform plastics into highly complex mixtures of chemicals with unknown fates and impacts. While plastics research to date has largely studied pure polymers, these results show that the various consumer plastics that are actually in the environment behave differently due to additives they contain. Therefore, understanding the fates and impacts of plastic pollution - and developing next generation materials that readily break down in the environment – will require a shift towards research that studies plastics that are more representative of those leaked into the environment.

**Why did this research need the NHMFL?** The 21 Tesla Fourier transform ion cyclotron resonance mass spectrometer offers the highest mass resolving power and mass accuracy in the world. This NHMFL magnet system allowed these NHMFL users to measure at least ten times more sunlight-produced compounds than others had observed using less powerful mass spectrometers.
BIO/MPS-DMR: CHEXS at CHESS - BioSAXS / HP Bio Beamline

- Biomolecular structure from solution
- High-pressure studies in biophysics
- Deep Life
- Food Science

Capabilities: High-throughput SAXS/WAXS, chromatography coupled SAXS (SEC-SAXS, AEX-SAXS), inline DLS/MALS, high-pressure SAXS (static sample to 700 MPa), high-pressure SEC-SAXS (100 MPa), mail-in program.

High Pressure Biology

HI-P SAXS and crystallographic facilities to examine the effects of Hi-P on the structure of biomolecules and elucidate the "rules of life" at the molecular level - a regime not currently accessible to biologists.

https://www.chess.cornell.edu/users/biosaxs-hp-bio-beamline
MPS/AST: NSF’s newest solar telescope produces first images, most detailed images of the sun

The Daniel K. Inouye Solar Telescope revealed unprecedented detail of the sun's surface and is enabling a new era of solar science and a leap forward in understanding the sun and its impacts on our planet.
THANK YOU!

lsapocha@nsf.gov

Directorate for Mathematical and Physical Sciences