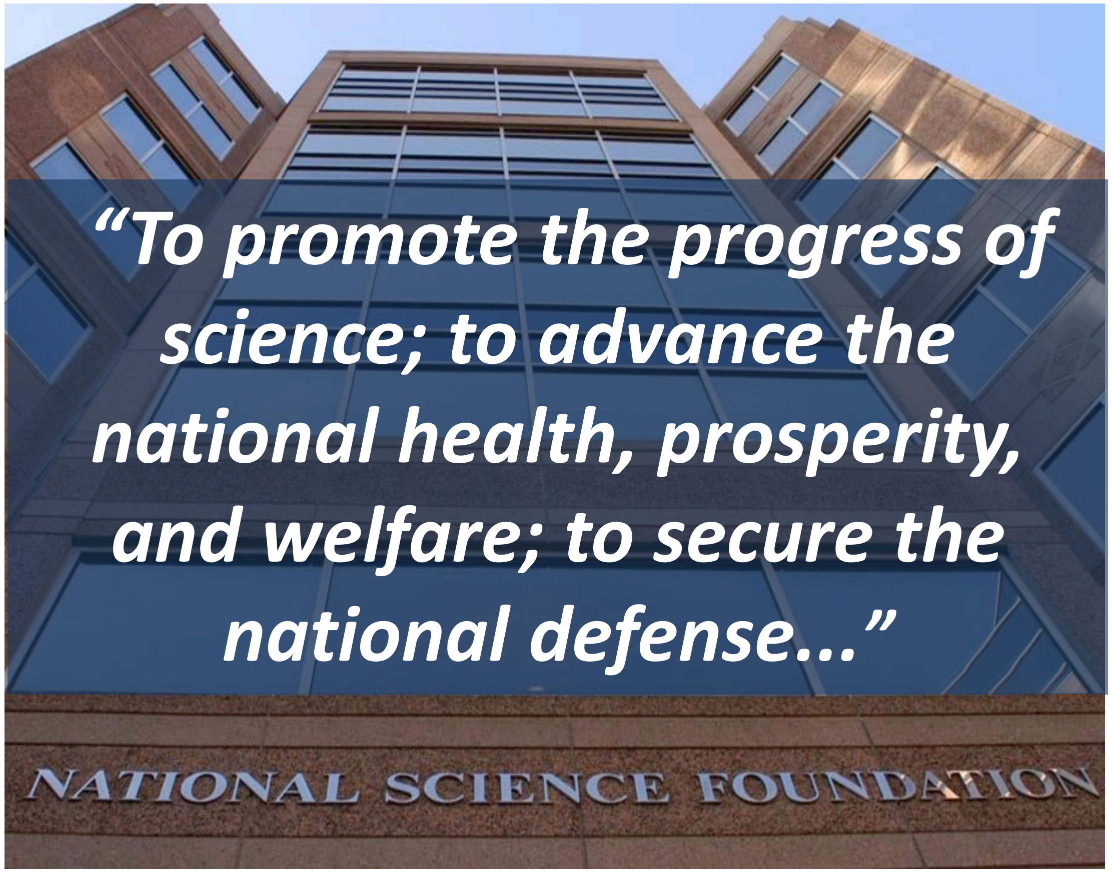
NSF Engineering Research Opportunities

DOE Fuel Cell Technologies Office Annual Merit Review and Peer Evaluation Meeting, June 14, 2018

Carole J. Read, Angela Lueking, Robert McCabe, and Triantafillos Mountziaris

NSF Mission



"To promote the progress of science; to advance the national health, prosperity, and welfare; to secure the national defense..."

Division of Chemical, Bioengineering, Environmental, and Transport Systems


Division Director
Richard Dickinson


Deputy Division Director
Timothy Patten

Chemical Process Systems


1401 Catalysis
Robert McCabe


1417 Molecular Separations
Angela Lueking


1403 Process Systems, Reaction Engineering, & Molecular Thermodynamics
Triantafillos Mountziaris


7644 Electrochemical Systems
Carole Read

Chemical Process Systems Cluster
VACANT

Engineering Biology & Health


1491 Cellular & Biochemical Engineering
Steven Peretti


5345 Engineering of Biomedical Systems
Michele Grimm


7236 Biophotonics
Leon Esterowitz


7909 Biosensing
Chenzhong Li


5342 Disability & Rehabilitation Engineering
Michele Grimm


Engineering Biology & Health Cluster
Christina Payne

Environmental Engineering & Sustainability


1440 Environmental Engineering
Karl Rockne


1179 Biological & Environmental Interactions of Nanoscale Materials
Nora Savage


7643 Environmental Sustainability
Bruce Hamilton


022Y INFEWS
James Jones


Environmental Engineering & Sustainability Cluster
Brandi Schottel

Transport Phenomena


1407 Combustion & Fire Systems
Song-Charng Kong


1443 Fluid Dynamics
Ronald Joslin


1415 Particulate & Multiphase Processes
Susan Muller


1406 Thermal Transport Processes
José Lage


Transport Phenomena Cluster
Shahab Shojaei-Zadeh

Division Experts and AAAS Science & Technology Policy Fellows


Multiple Programs Expert
Geoffrey Prentice


Engineering of Biomedical Systems Expert
Carol Lucas


AAAS S&T Policy Fellow
Gregory Meyer

Clean Energy Topics in CPS

- Investments in fundamental engineering science research including:
  - solar energy OPVs, solar fuels
  - biofuels and bioenergy
  - energy storage—batteries and flow batteries
  - fuel cells
  - energy efficiency
  - energy materials and manufacturing

Chemical Process Systems

Robert McCabe

Catalysis

- Heterogeneous catalysis related to sustainability and chemical processes
- Heterogeneous catalyst design, synthesis, and characterization
- Basic understanding of catalytic reactions, kinetics, and mechanisms

Angela Lueking

Molecular Separations

- Methods and mechanisms for purification of gases, chemicals, or water
- Mass separation agents or processes
- Field (flow, magnetic, electrical) induced separations

T.J. (Lakis) Mountziaris

Process Systems, Reaction Eng. & Mol. Thermodynamics

- Chemical Reaction Engineering
- Process Design, Optimization and Control
- Reactive Polymer Processing
- Molecular Thermodynamics for Chemical Processing and Materials

Carole Read

Electrochemical Systems

- Electrochemical Energy Systems
- Organic Photovoltaics

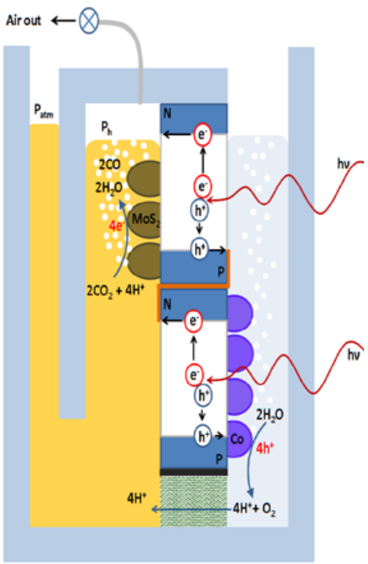
Robert McCabe

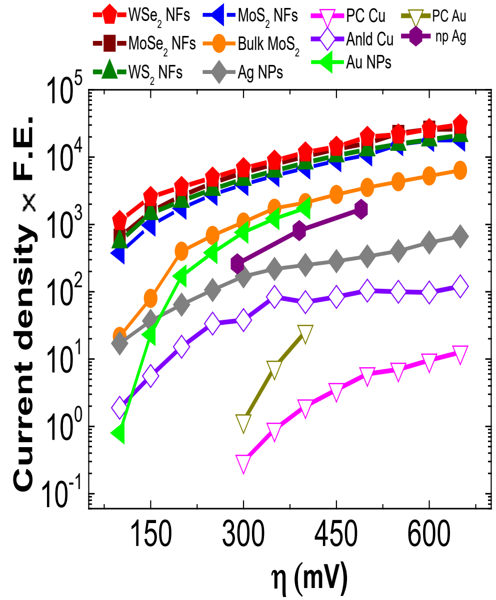
Directions for Catalysis Study:

- Basic understanding of catalytic mechanisms via kinetic studies, computational methods, and characterization techniques.
- Discovery, design, and synthesis of catalysts specifically tailored to lower activation barriers and promote high rates and desired selectivity.
- Scalable, economical, and durable catalyst formulations and synthesis methods targeted at applications of both long-term commercial and societal importance.

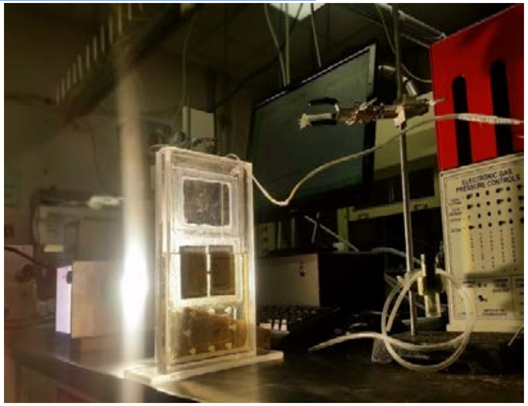
Artificial Leaf Platform; remarkable CO2 conversion performance

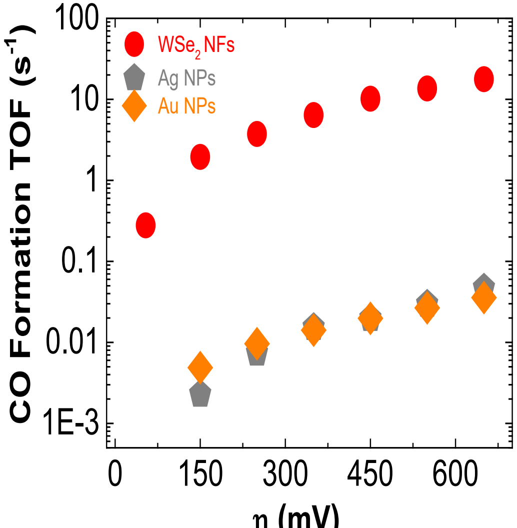
Dichalcogenide nanoflakes reduce CO_2 to CO electrochemically in an ionic liquid medium concurrently with an artificial leaf platform that oxidizes H_2O to O_2





Slide courtesy of Amin Salehi-Khojin





Partial support under NSF CBET - 1512647

M. Asadi, K. Kim, C. Liu, A.V. Addepalli, P. Abbasi, P. Yasaei, P. Phillips, A. Behranginia, J.M. Cerrato, R. Haasch, P. Zapol, B. Kumar, R.F. Klie, J. Abiade, L.A. Curtiss, and **A. Salehi-Khojin**. *Science*, (**2016**) [DOI: 10:1126/science.aaf4767].

Carole J. Read

Electrochemical Systems Program FY18

Program Goals:

- Support fundamental engineering research that will enable innovative processes for the sustainable production of electricity, fuels, and chemicals and for energy storage.
- Stress molecular level understanding of phenomena that directly impacts key barriers to improved system level performance (e.g. energy efficiency, product yield, process intensification)
- Proposed research should be inspired by the need for economic and impactful conversion processes.

Electrochemical Systems FY18 Themes

Electrochemical Energy Systems:

- Energy storage for renewable electricity production & transport
- Solar fuels: Photocatalytic or photoelectrochemical processes for the splitting of water into H2 gas, or for the reduction of CO2 to liquid or gaseous fuels
- Fuel Cells and Electrochemical chemicals

Organic Photovoltaics (OPVs):

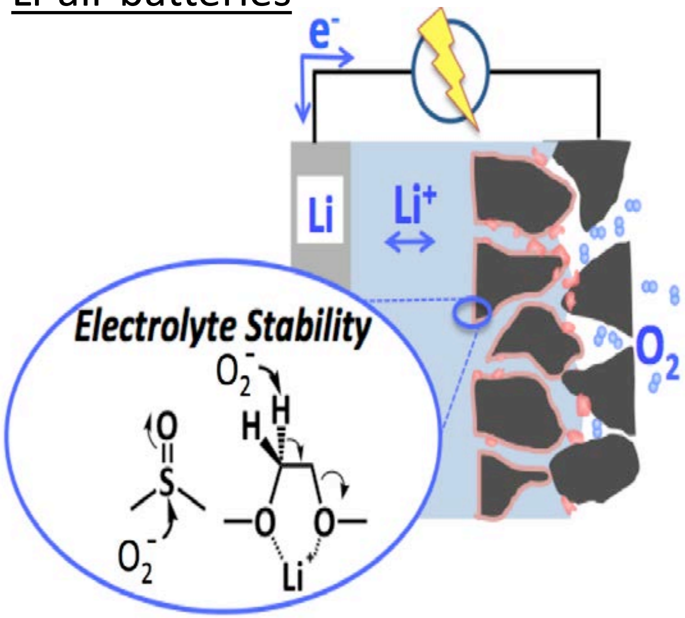
- Fundamental research on innovative processes for the fabrication and theory-based characterization of future organic PV devices
- Devices of interest include polymer and small molecule OPVs for electricity generation

CAREER: Novel redox-active electrolyte additives to enhance efficiency and direct product selectivity in electroreduction reactions

Bryan McCloskey, University of California-Berkeley, CBET-1653430 (Start Date: July 2017)

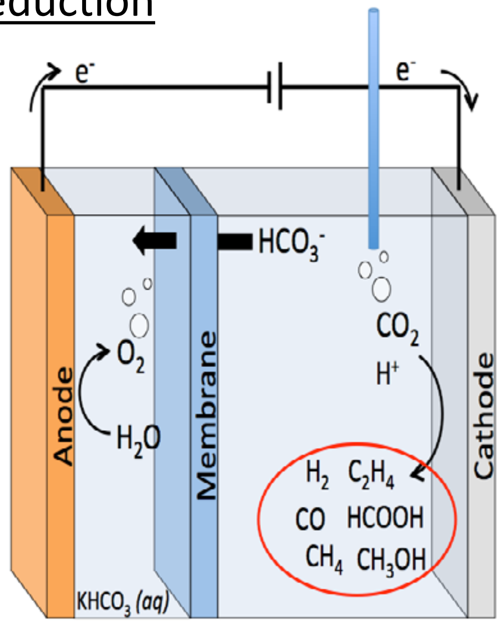
Overall goal: Improve desirable product selectivity during O_2 and CO_2 reduction

Li-air batteries



Challenge: Reduced oxygen species degrade electrolyte

CO_2 reduction



Challenge: Poor product selectivity and energy efficiency

Approach: Identify and incorporate electrolyte additives to promote desired reactions

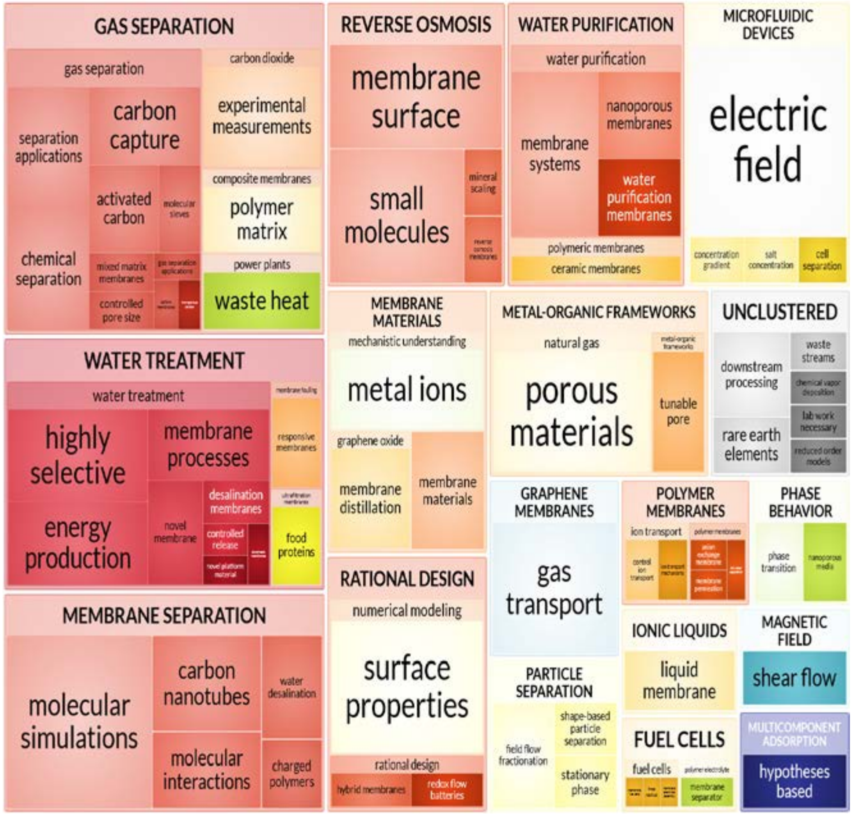
Preliminary research indicates that adding soluble redox-active molecules to the electrolyte can dramatically influence product distributions in Li-air batteries and during CO_2 reduction. We will specifically pursue the use of N-heterocycles to promote desired reactions in these systems, stressing elucidation of reaction mechanisms to understand how to appropriately design electrolytes that improve each systems' performance.

Angela Lueking

Molecular Separations

The Molecular Separations program supports research focused on **novel methods and materials** for **separation processes**, such as those central to the chemical, biochemical, bioprocessing, materials, energy, and pharmaceutical **industries**.

A **fundamental understanding** of the **interfacial, transport, and thermodynamic behavior of multiphase chemical systems** as well as **quantitative descriptions of processing characteristics** in the process-oriented industries is critical for efficient resource management and effective environmental protection.

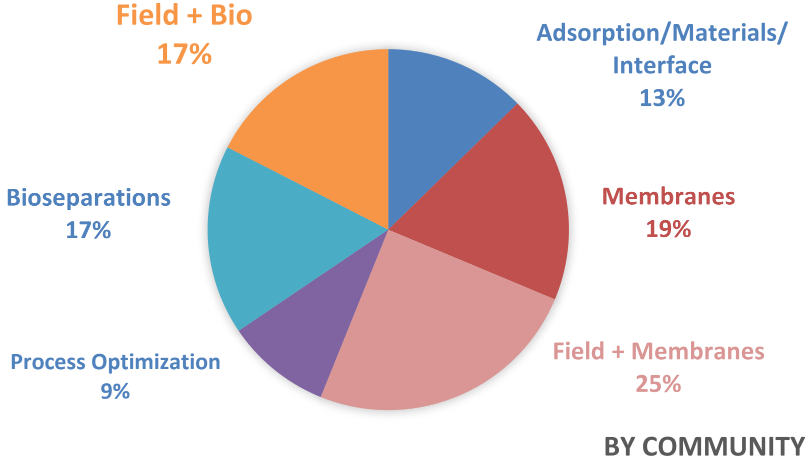


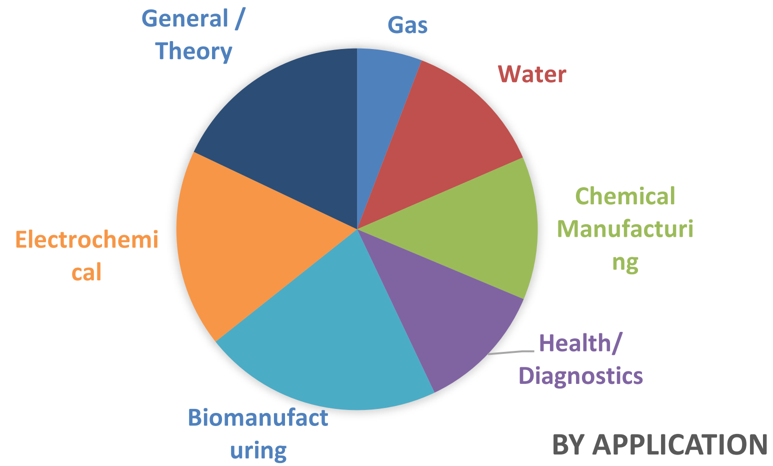
A snapshot of proposals submitted since July 2017

Molecular Separations

Areas of emphasis (FY18):

- Design of scalable mass separating agents and/or a mechanistic understanding of the interfacial thermodynamics and transport phenomena that relate to purification of gases, chemicals, or water
- Design or improvement of mass separation agents or processes that are based upon, and advance, transport principles
- Downstream purification of biologically derived chemicals for increased throughput
- Field (flow, magnetic, electrical) induced separations and other innovative approaches that address a significant reduction in energy and/or materials requirements in the process industries





A snapshot of unsolicited awards in FY2017

T.J. Mountziaris

Process Systems, Reaction Engineering and Molecular Thermodynamics (PRM)

Program supports research and education projects related to:

1. Interactions between chemical reactions and transport phenomena in reactive systems, and the use of this information in the design of complex chemical and biochemical reactors (**Reaction Engineering**)

   a. Reactive processing of polymers, ceramics, and thin films

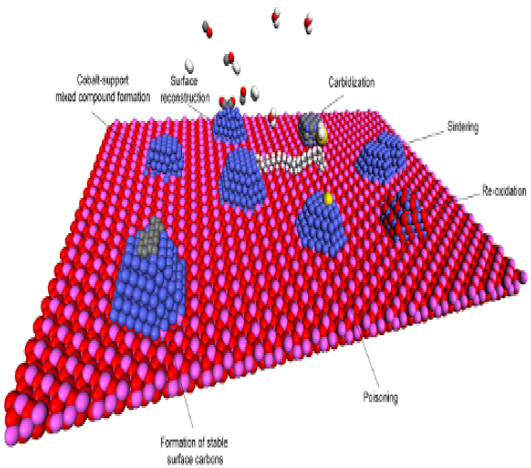
   b. Electrochemical and photochemical processes of engineering significance or with commercial potential

2. Design and optimization of complex chemical processes (**Design**)
3. Dynamic modeling and control of process systems and individual process units (**Control**)
4. New materials and processes based on utilizing Molecular Simulation and Statistical Thermodynamics (**Molecular Thermodynamics**)

NSF-DOE Workshop: Modular Manufacturing

➢ **Investments in fundamental engineering science research including:**

- **process intensification**
- **modular reactors**
- **energy efficiency**
- **systems controls**



Molecular-level Science and Engineering

Module-level Integration

Pilot Scale

Plant Scale

NSF Funded Projects

Projects funded by Mission-Oriented Agencies (e.g., DOE)

http://www.efrc.udel.edu/2017NSFWorkshop/

Advice… Talk to a friendly program officer

Determining program fit takes homework

- Write up a 1-pager
    - Have your overview paragraph,
    - Intellectual merit paragraph
    - Broader impacts paragraph

- Make clear what is your transformative feature of your research and why
- Email 1-pager to program officer and ask for input
- In the end, it is your choice where to submit

Moved to Alexandria, Virginia ☹

Contacts and Thank you for Serving as a Reviewer!

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Lakis Mountziaris
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tmountzi@nsf.gov

Chemical Process Systems Cluster

Chemical processes are critical in the production of chemicals, materials, clean water, energy, pharmaceuticals, and other commodities. The Chemical Process Systems (CPS) Cluster has four programs that **support fundamental science and engineering research for the development of novel materials, mechanisms, and/or tools to improve the efficiency, resource utilization, and/or intensification of chemical processes**. This cluster supports research seeking innovations in catalytic design, reaction engineering, multiphase chemical separations processes, molecular thermodynamics, process control and design, and sustainable energy conversion.

The overarching goal of the CPS programs is to support basic research that improves the overall efficiency and product yields of chemical processes while reducing the size and complexity of process equipment and minimizing emissions.