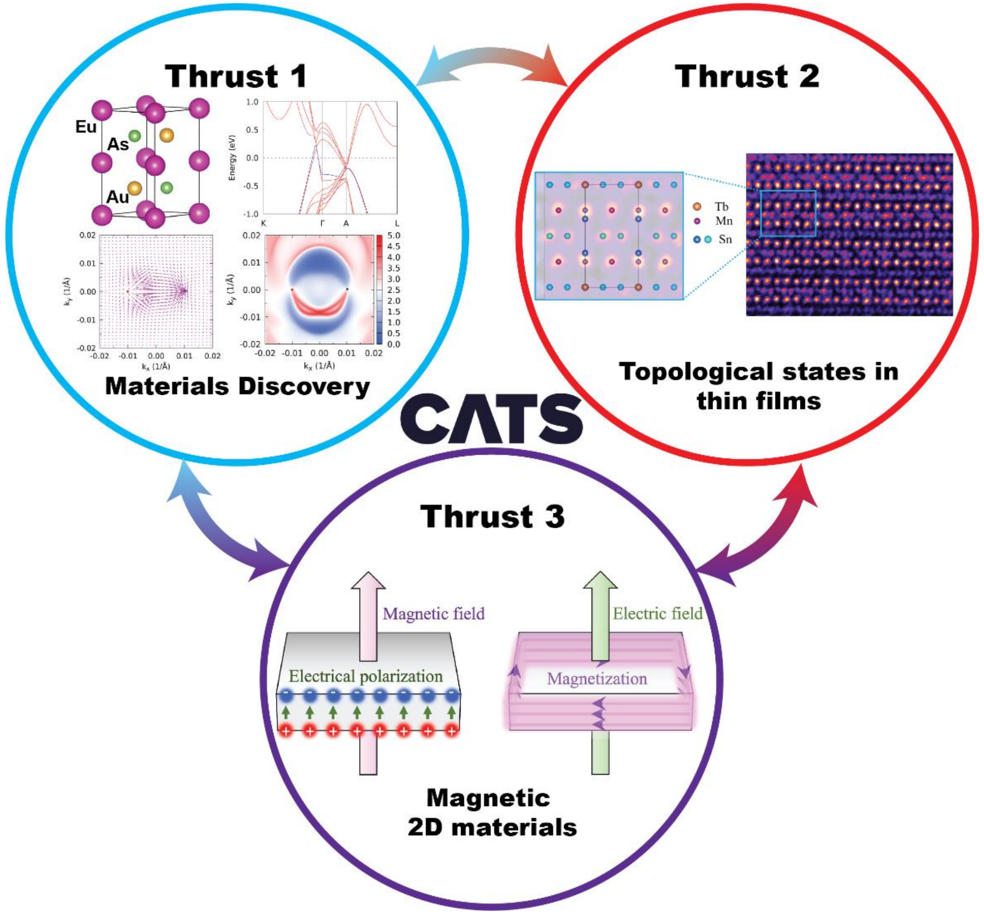
Center for the Advancement of Topological Semimetals (CATS)

Robert McQueeney (Ames National Laboratory); Class: 2018-2026

MISSION: To transform how we discover, understand, and harness new topological states of matter.

RESEARCH PLAN

CATS has three Research Thrusts: **(1)** ***Discovery and control of magnetic and correlated topological matter*** emphasizes the discovery of new magnetic topological materials; **(2)** ***Novel topological states in thin films*** recognizes the importance of developing films for delivery of controllable quantum transport in topological materials; and **(3)** ***Topological magnetism and magnetoelectricity in 2D materials*** focuses on emergent properties of highly tunable vdW assemblies.



http://cats.ameslab.gov

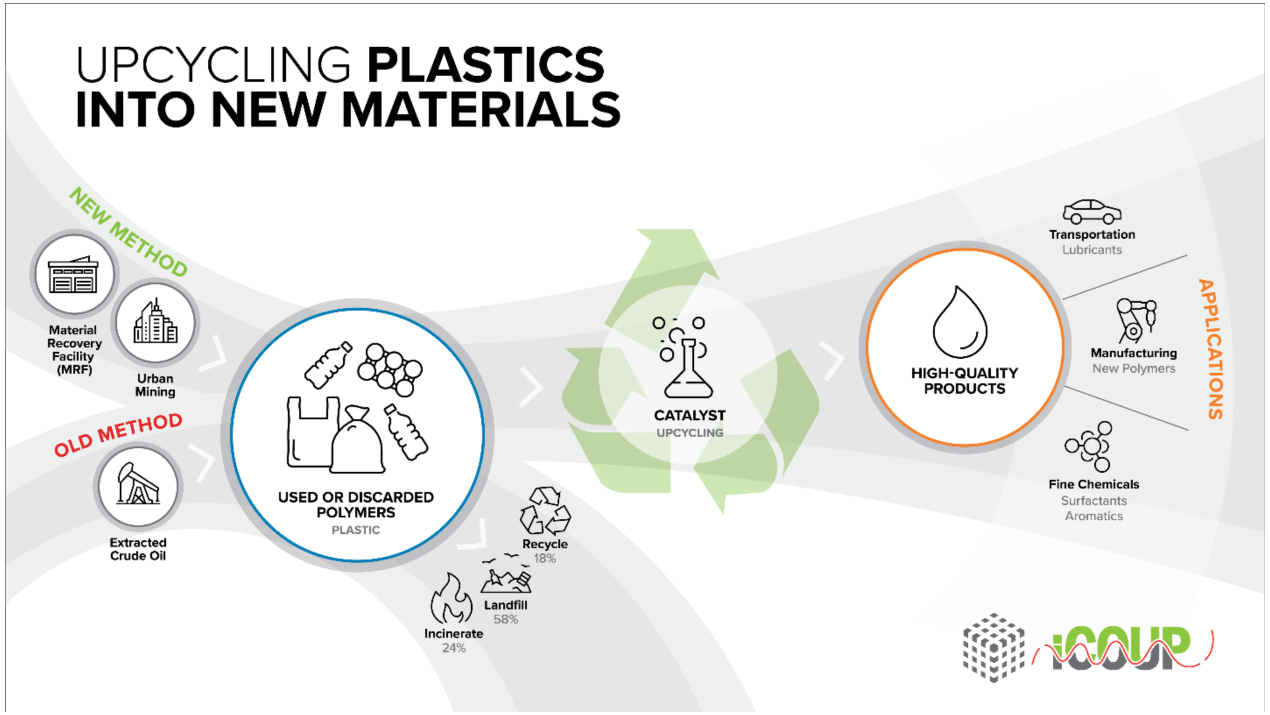
AMES NATIONAL LABORATORY Creating Materials & Energy Solutions · Argonne NATIONAL LABORATORY · BOSTON COLLEGE · HARVARD UNIVERSITY · UC SANTA BARBARA · Massachusetts Institute of Technology · CATS · Los Alamos NATIONAL LABORATORY · UIC UNIVERSITY OF ILLINOIS CHICAGO · UNIVERSITY OF WATERLOO

U.S. DEPARTMENT OF ENERGY | Office of Science

Institute for Cooperative Upcycling of Plastics (iCOUP)

Aaron Sadow (Ames National Laboratory); Class: 2020-2024

MISSION: To uncover macromolecular and catalytic phenomena at the interface of molecular-scale chemistry and mesoscale materials science in order to enable upcycling of energy-rich plastics.



https://www.ameslab.gov/institute-for-cooperative-upcycling-of-plastics-icoup

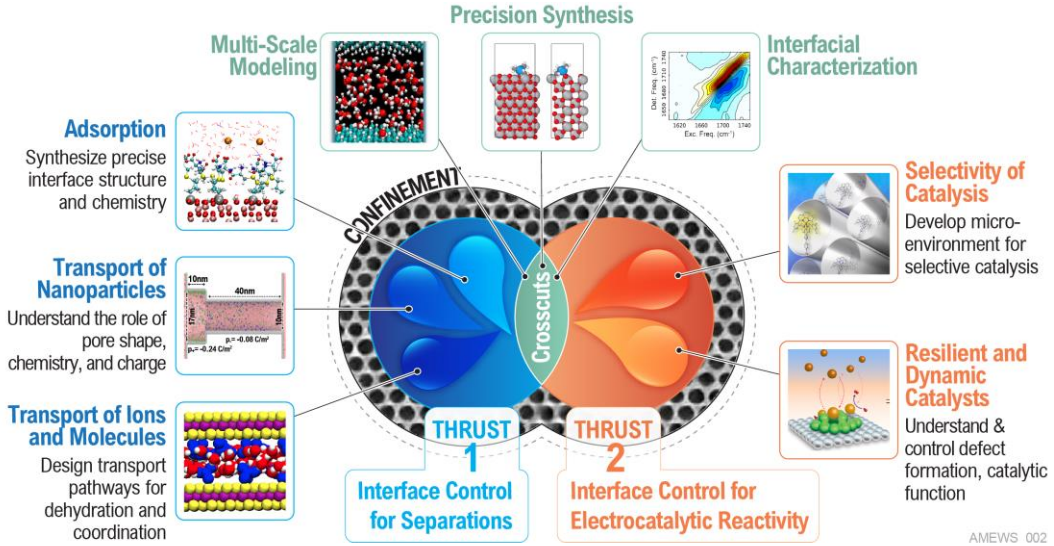
RESEARCH PLAN

We are creating inorganic catalysts to cleave specific bonds in polyolefins, discovering new methods for polymer upcycling into value-added products and materials, and understanding the phenomena, such as macromolecule-catalyst interactions, underpinning these transformations.

Advanced Materials for Energy-Water Systems (AMEWS)

Seth Darling (Argonne National Laboratory); Class: 2018-2026

MISSION: To revolutionize our understanding of aqueous solutes in confined and electrified environments at interfaces, by integrating new experimental, theoretical, and modeling capabilities.



https://www.anl.gov/amews

RESEARCH PLAN

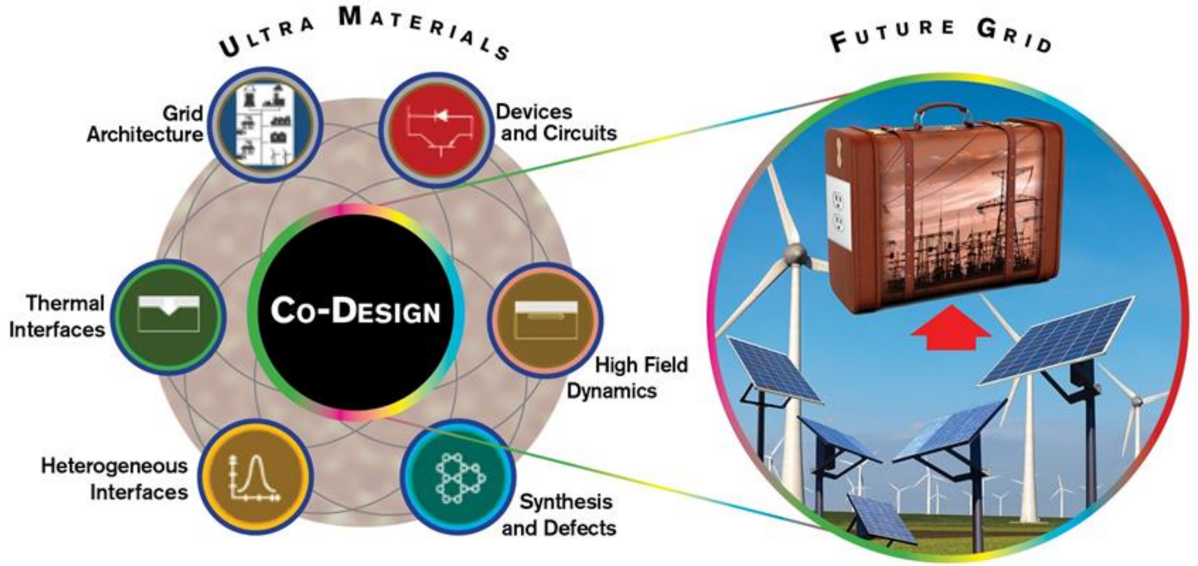
Our goals are to:

1. Design and control transport properties of ions, molecules, and nanoparticles under confinement
2. Discover pathways to capture and control release of trace solutes from complex aqueous solutions
3. Identify new mechanisms to drive selective electrocatalysis in complex aqueous mixtures
4. Predict and synthesize catalysts that are resilient under electro-active aqueous environments

Ultra Materials for a Resilient, Smart Electricity Grid (ULTRA)

Robert J. Nemanich (Arizona State University); Class: 2020-2024

MISSION: To achieve extreme electrical properties and phenomena through fundamental understanding of ultra wide bandgap materials – including synthesis and impurity incorporation, electronic structure at interfaces, electron - phonon interactions at high fields, and phonon mediated thermal transport, which will enable a resilient, smart electricity grid.



https://ultracenter.asu.edu/

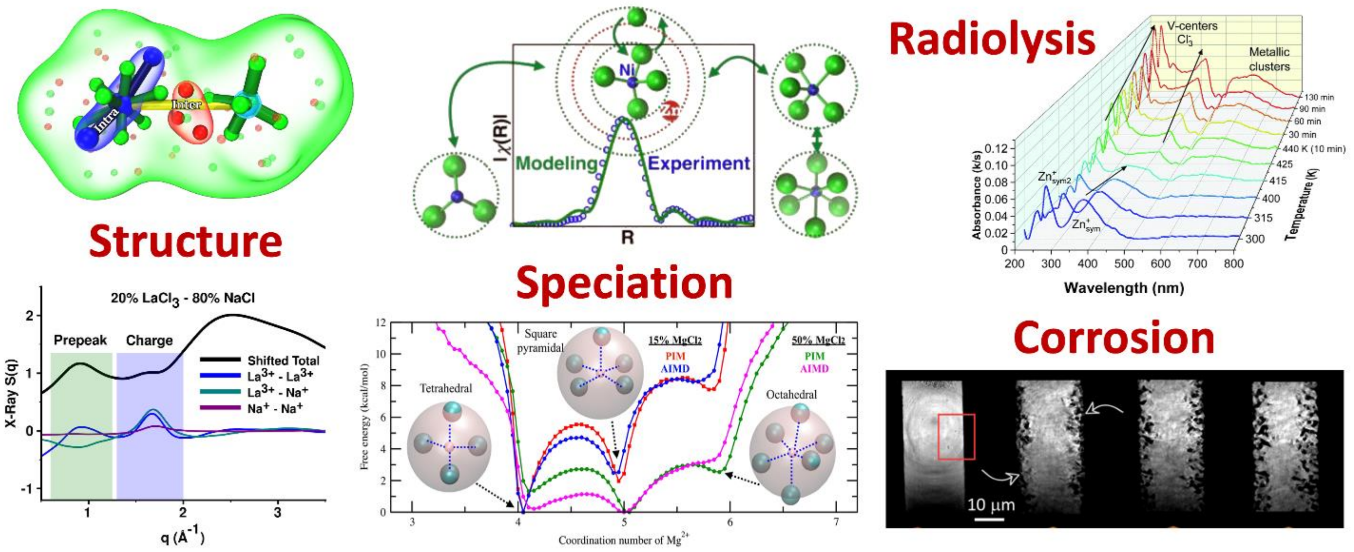
RESEARCH PLAN

Specific outcomes will include: 1) synthesis of cubic and hexagonal ultra semiconductors, 2) experimental and theoretical understanding of defects and doping that transcends the materials systems, 3) characterized ultra heterostructures enabling new routes to doping, 4) understanding electric breakdown phenomena and high current transport in ultra semiconductors, and 5) characterized interactions between electrons and phonons in ultra materials and importantly, their interfaces.

Molten Salts in Extreme Environments (MSEE)

James Wishart (Brookhaven National Laboratory); Class: 2018-2026

MISSION: To provide fundamental and predictive understanding of molten salt bulk and interfacial chemistry that will establish robust principles to guide the technologies needed to deploy molten salt nuclear reactors.



https://www.bnl.gov/moltensalts

RESEARCH PLAN

MSEE combines cutting-edge experimental capabilities for high-temperature research with a unified computational effort performing molten salt simulations to examine the atomic basis of molten salt behavior and provide a predictive description of molten salt chemistry under the coupled extremes of high temperature and ionizing radiation.

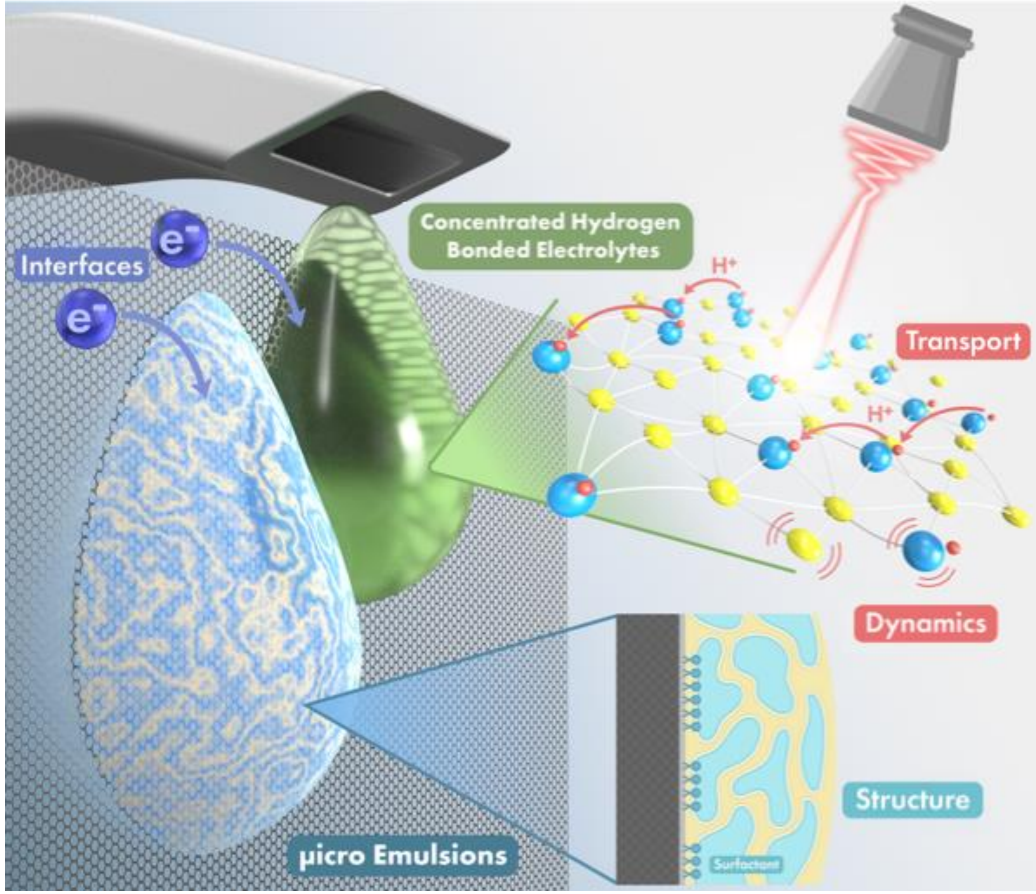
Breakthrough Electrolytes for Energy Storage and Systems (BEES2)

Robert Savinell (Case Western Reserve University); Class: 2018-2026

MISSION: To uncover the transport mechanisms of ions, protons, redox species, and electrons in nano to meso scale structured electrolytes in the bulk and at the electrode-electrolyte interfaces to achieve high energy and power density in next generation energy storage systems.

RESEARCH PLAN: BEES2 aims to advance electrolytes discovery to achieve safer and more efficient performance in the next generation energy storage and chemical transformation technologies that are critical for decarbonization and storage of energy harvested from sunlight, wind, and other renewables.

An integrated research approach utilizing team expertise in electrochemistry, synthesis, modeling and theory, and physical/chemical structure and property characterization is employed to explore the electrolyte science.



https://engineering.case.edu/research/centers/breakthrough-electrolytes-for-energy-storage

BEES2

Case Western Reserve University EST. 1826

Pacific Northwest National Laboratory

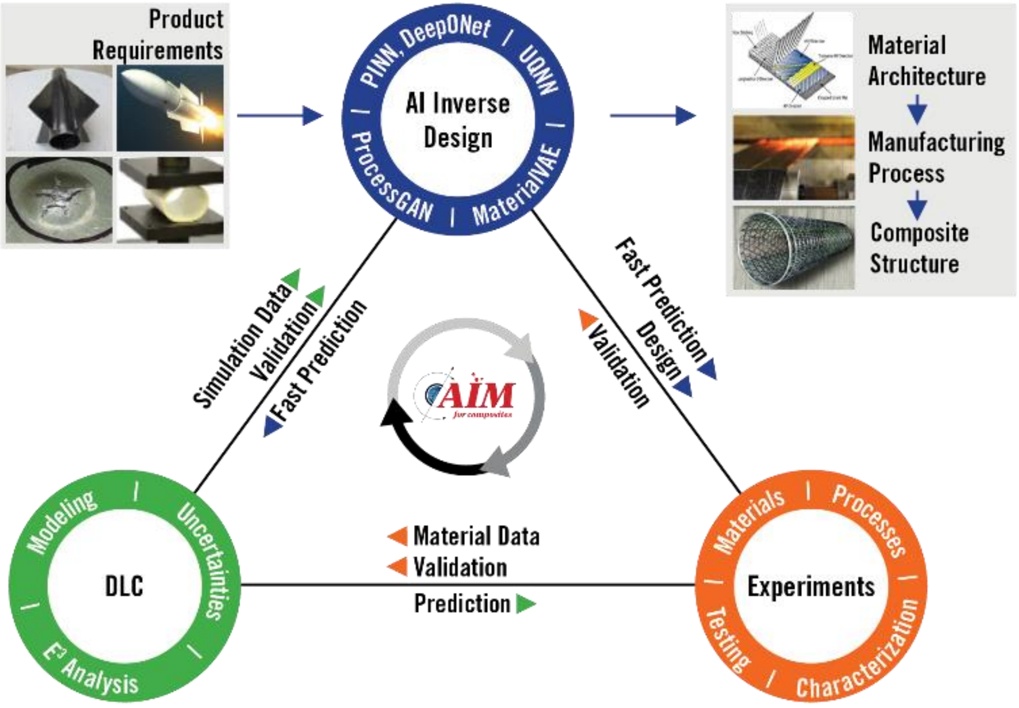
Artificially Intelligent Manufacturing Paradigm for Composites (*AIM for Composites*)

Srikanth Pilla (Clemson University); Class: 2022-2026

MISSION: To build an AI-enabled inverse design approach for fundamental understanding and integrated material-manufacturing design of advanced polymer composites.

RESEARCH PLAN

AIM for Composites brings together a multi-disciplinary team of experimentalists, computational researchers, and computer scientists to (1) unravel the fundamental underpinnings of the material-process-microstructure-performance (MP2) relationship via constructing a "Digital Life Cycle" (DLC) high fidelity multiscale modeling and simulation platform; (2) leverage physics-informed AI models to enable inverse composites material architecture and manufacturing process design; and (3) inform and validate the DLC and AI models and implement new material and process designs by exploiting innovative material engineering, characterization, and testing methods.



https://clemson.edu/efrc

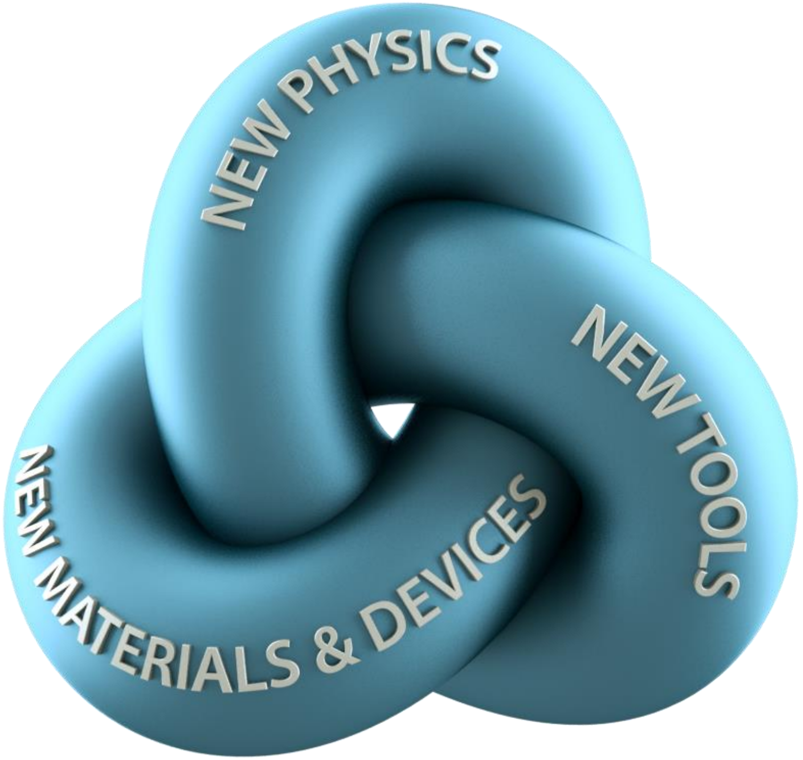
Programmable Quantum Materials (Pro-QM)

D.N Basov (Columbia University); Class: 2018-2026

MISSION: To discover, characterize and deploy new forms of quantum matter controllable by light, gating, magnetic proximity electromagnetic environment, and nano-mechanical manipulation, effectively programming their quantum properties.

RESEARCH PLAN

Realizing the potential for programmable quantum matter requires a three-pronged approach, combining *i)* the unique suite of controls and driving perturbations with *ii)* a transformative set of synthesis/device fabrication capabilities and *iii)* new nanoscale characterization techniques integrated in a single platform.



https://quantum-materials.columbia.edu

Pro-QM
Programmable Quantum Materials
DOE Energy Frontiers Research Center

U.S. DEPARTMENT OF ENERGY | Office of Science

COLUMBIA UNIVERSITY IN THE CITY OF NEW YORK

Brookhaven National Laboratory

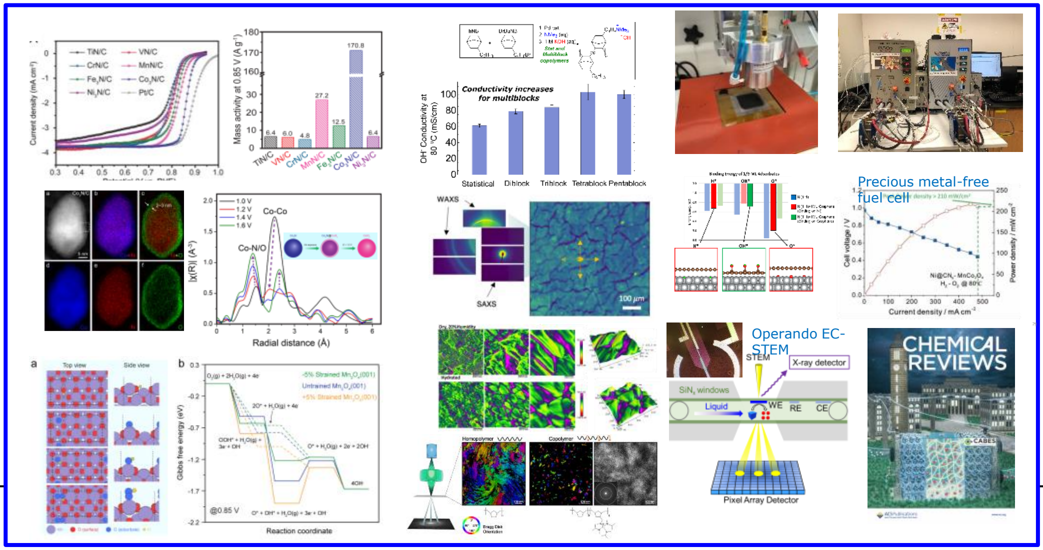
Center for Alkaline Based Energy Solutions (CABES)

Héctor D. Abruña (Cornell University); Class: 2018-2026

MISSION: To advance the scientific understanding of the fundamental factors governing electrocatalysis and electrochemical energy conversion in alkaline media.

CABES
Center for Alkaline-based Energy Solutions

www.cabes.cornell.edu



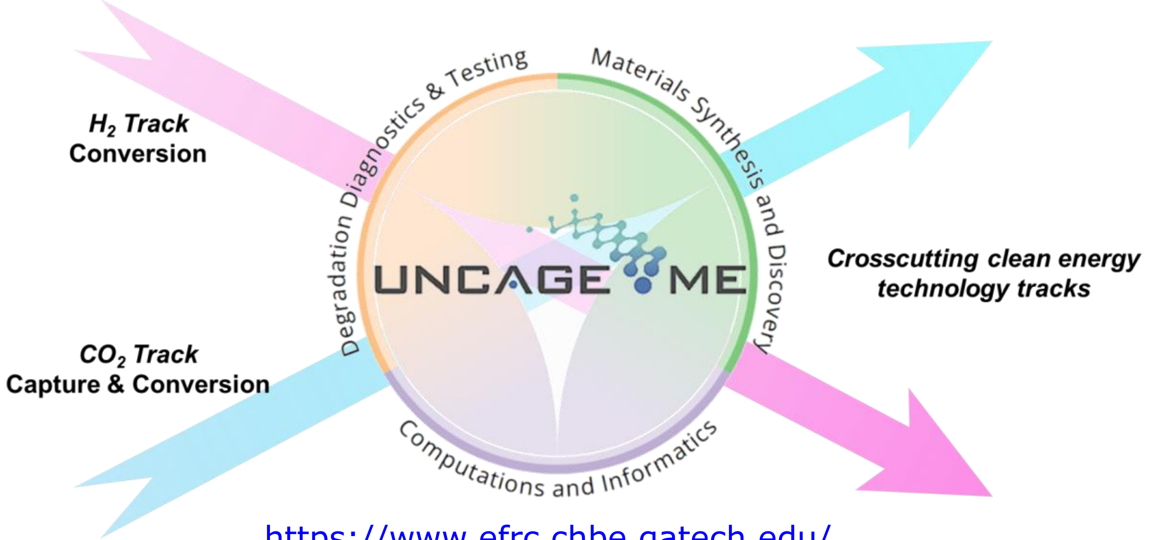
RESEARCH PLAN

Alkaline media enables electrochemical energy conversion technologies that utilize only abundant elements. The **Center for Alkaline Based Energy Solutions *(CABES)*** is establishing, via three ***Fundamental Science Drivers,*** (1.What factors govern electrocatalysis in alkaline media? 2.How do we understand and control transport in alkaline media? 3.What makes energy materials durable in alkaline media?) a comprehensive description of the nature, structure, and dynamics of electrocatalysis in alkaline media via an integrated research approach that includes theory and computational methods, synthesis of electrocatalysts and novel membrane materials and the development of novel experimental tools to provide *in situ/operando*, spatiotemporal characterization of systems under operation.

Understanding and Controlling Accelerated and Gradual Evolution of Materials for Energy (UNCAGE-ME)

Ryan Lively (Georgia Institute of Technology); Class: 2014-2026

MISSION: To develop a deep knowledge base in the characterization, prediction, and control of materials evolution in the presence of realistic contaminants, processes, and mixtures to accelerate materials discovery for sustainable production and utilization of H_2 and CO_2.



https://www.efrc.chbe.gatech.edu/

RESEARCH PLAN

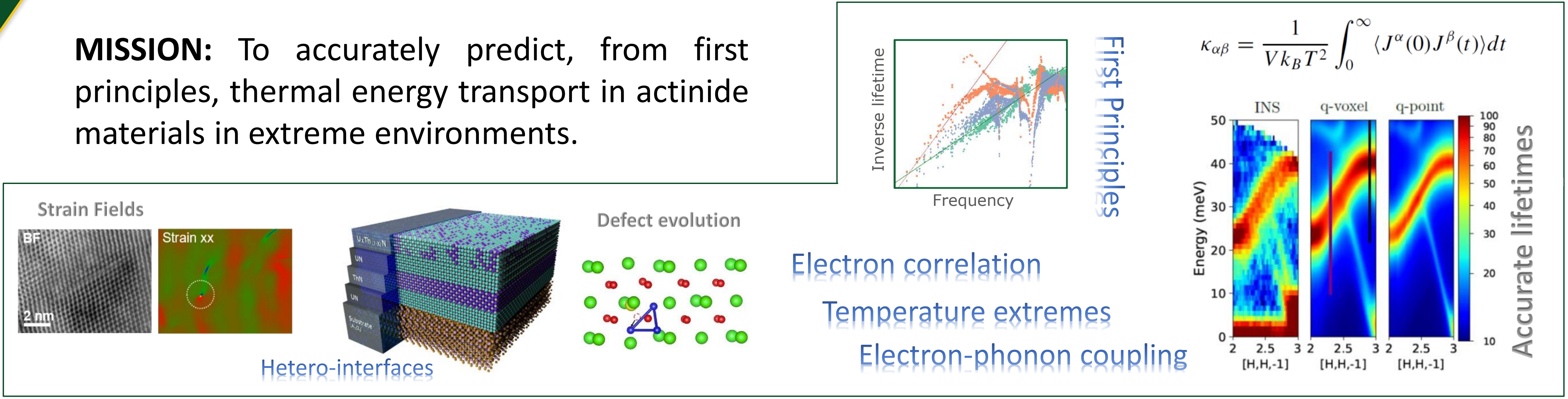
1) Elucidate the overarching relationships for process-induced structure and property evolution of functional materials with a focus on separations media and (electro)catalysts. 2) Leverage and advance computational and machine learning techniques to enable fundamental molecular and electronic level predictions of materials interacting with complex mixtures of targeted gases and contaminants. 3) Demonstrate accelerated materials discovery for clean energy technologies via process-materials coupled research.

UNCAGE ME · Georgia Tech · Sandia National Laboratories · Lehigh University · UC Riverside · The University of Alabama · University of Michigan · University of Florida · Oak Ridge National Laboratory

Center for Thermal Energy Transport under Irradiation (TETI)

David Hurley (Idaho National Laboratory); Class: 2018-2026

MISSION: To accurately predict, from first principles, thermal energy transport in actinide materials in extreme environments.



http://teti.inl.gov

RESEARCH PLAN

Thermal energy transport in nuclear fuel is directly related to fuel performance, safety margins, and fuel longevity. The aim of TETI is to develop a first principles understanding of electron and phonon transport in advanced nuclear fuels that will provide the necessary tools to enhance thermal transport by tailoring defects and microstructure.

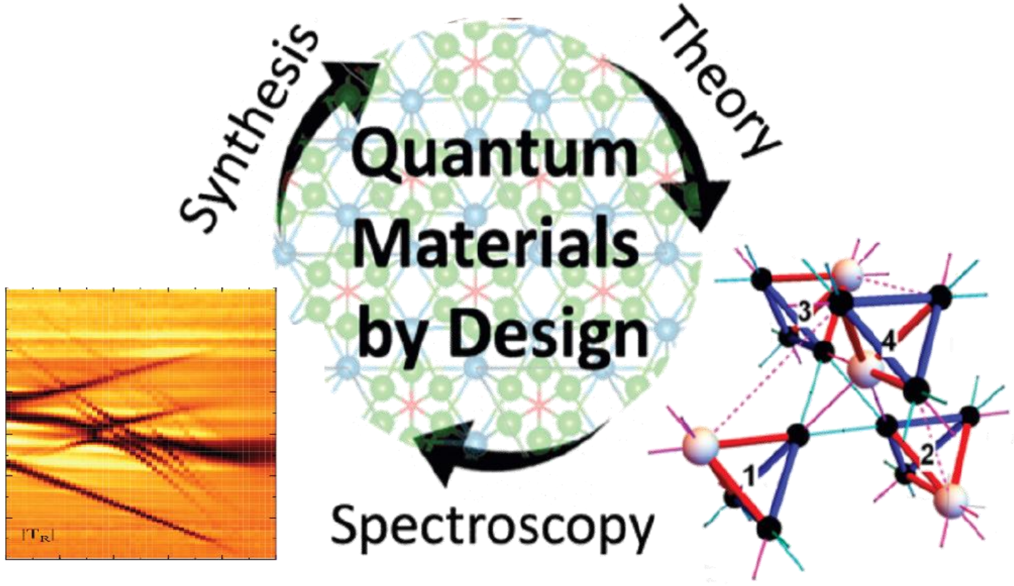
Institute for Quantum Matter (IQM)

Collin Broholm (Johns Hopkins University); Class: 2018-2024

Mission: To realize, understand, and control revolutionary quantum materials and structures where quantum effects such as entanglement and coherence find collective macroscopic manifestations.

RESEARCH PLAN

Quantum mechanics successfully describes electrons within atoms as matter waves. IQM will develop "Quantum Materials" where electronic matter waves extend beyond the atomic scale and give rise to unique physical properties. IQM theorists will identify candidate materials and nanoscale structures that will be synthesized and then probed with advanced spectroscopic and transport methods to realize and understand new quantum states of matter and explore their potential for applications.

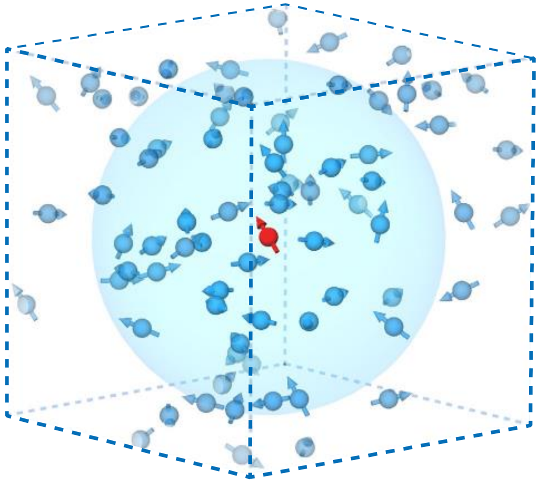


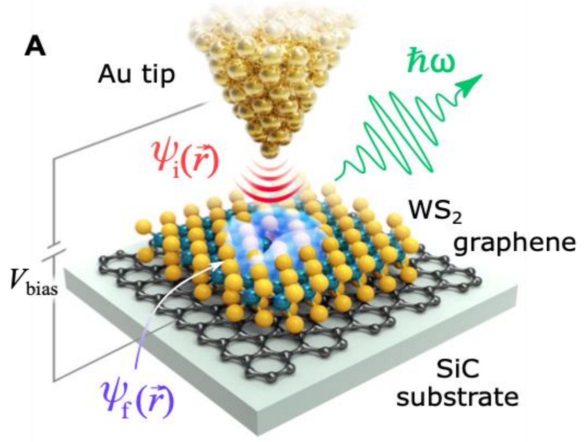
https://iqm.jhu.edu

Center for Novel Pathways to Quantum Coherence in Materials (NPQC)

Joel E. Moore (Lawrence Berkeley National Laboratory); Class: 2018-2024

MISSION: To expand dramatically our understanding and control of coherence in solids by building on recent discoveries in quantum materials along with advances in experimental and computational techniques.





http://npqc.lbl.gov

RESEARCH PLAN

NPQC studies families of materials in which quantum coherence is especially important using a variety of advanced characterization techniques and theoretical methods. Major outcomes include new approaches to solid-state quantum sensing and quantum spectroscopy, along with controllable coherent and incoherent transport behavior enabled by the creation of nanoscale interfaces and devices.

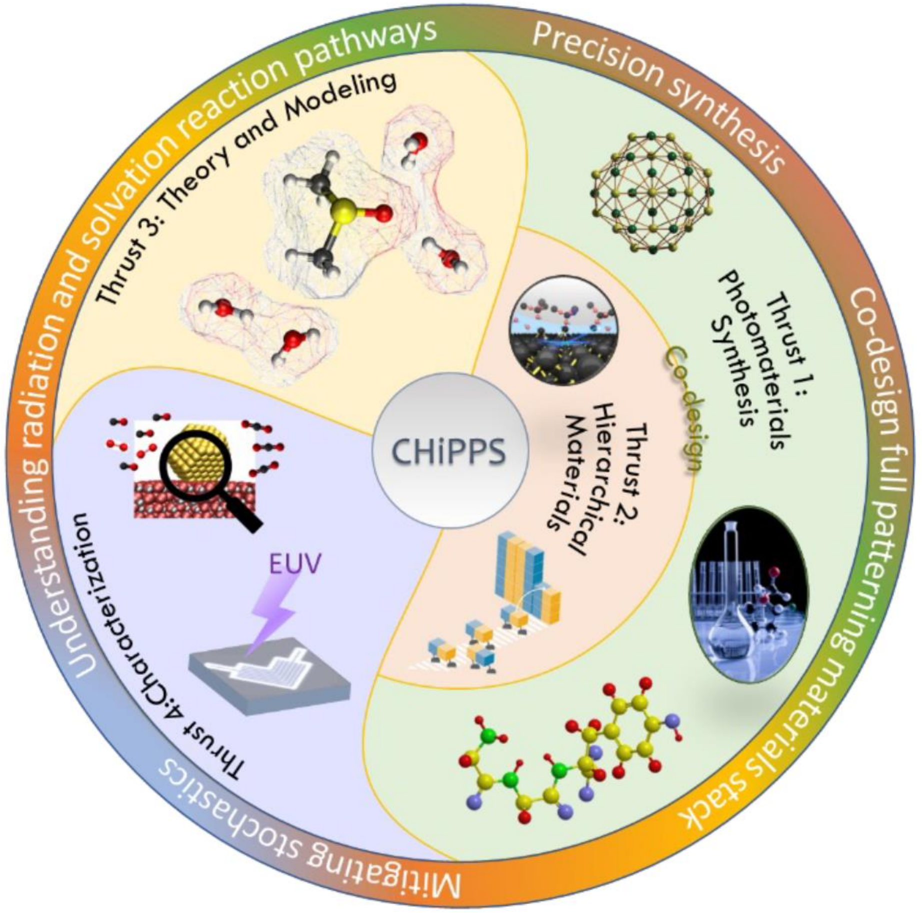
HARVARD UNIVERSITY UCSB Argonne NATIONAL LABORATORY BERKELEY LAB npqc

U.S. DEPARTMENT OF ENERGY | Office of Science

Center for High Precision Patterning Science (CHiPPS)
Ricardo Ruiz (Lawrence Berkeley National Laboratory); Class: 2022-2026

MISSION: To create new fundamental understanding and control of patterning materials and processes for energy-efficient, large-area patterning with atomic precision, thereby enabling at-scale advanced manufacturing of future generation microelectronics such as quantum and spin-based memory, storage, and logic devices.

RESEARCH PLAN: CHiPPS addresses the grand challenges in patterning science by developing a comprehensive understanding of how to efficiently harness high energy photons to perform selective chemical reactions in multifunctional radiation-sensitive materials while mitigating detrimental stochastic variability. This new understanding and control will be achieved through a holistic approach synergistically combining advances in co-designed materials synthesis, processing, self-assembly, data-driven modeling, and advanced characterization in order to realize atomically-precise patterning at the nanoscale.

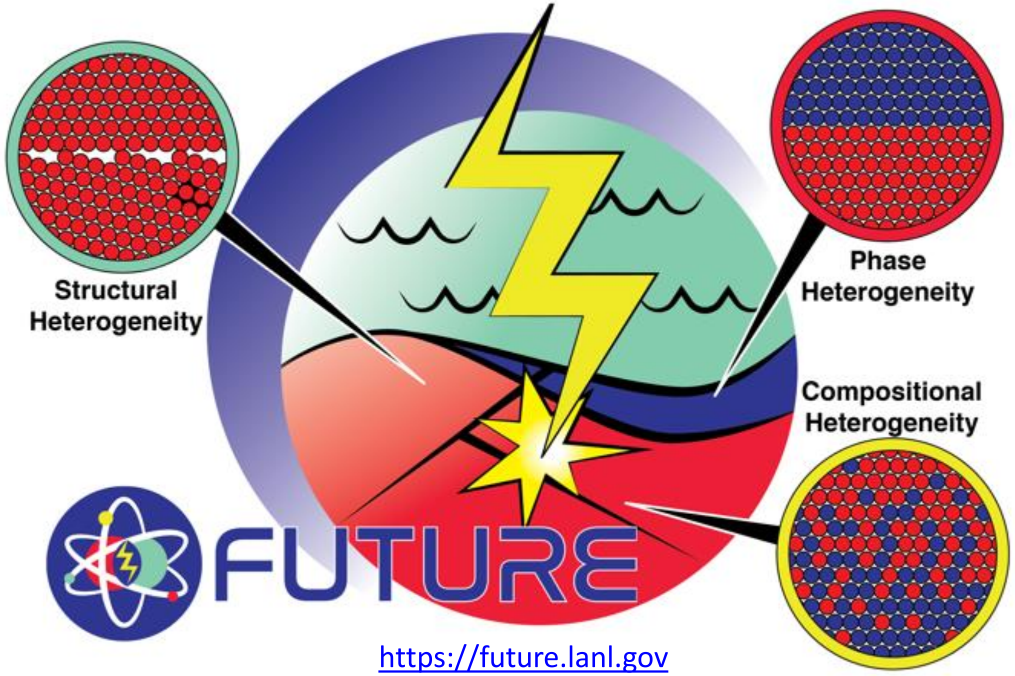


https://chipps.lbl.gov/

Fundamental Understanding of Transport Under Reactor Extremes (FUTURE)

Blas Pedro Uberuaga (Los Alamos National Laboratory); Class: 2018-2026

MISSION: To understand how the coupled extremes of irradiation and corrosion work in synergy to modify the evolution of materials by coupling experiments and modeling that target fundamental mechanisms.



https://future.lanl.gov

RESEARCH PLAN

The goal of FUTURE is to reveal the fundamental factors dictating the evolution of materials under the combined extremes of irradiation and corrosion to enable a descriptive and ultimately predictive understanding of these coupled extreme environments. We target the heterogeneities in structure, phase, and composition that define real-world materials that govern the irradiation and corrosive evolution of materials.

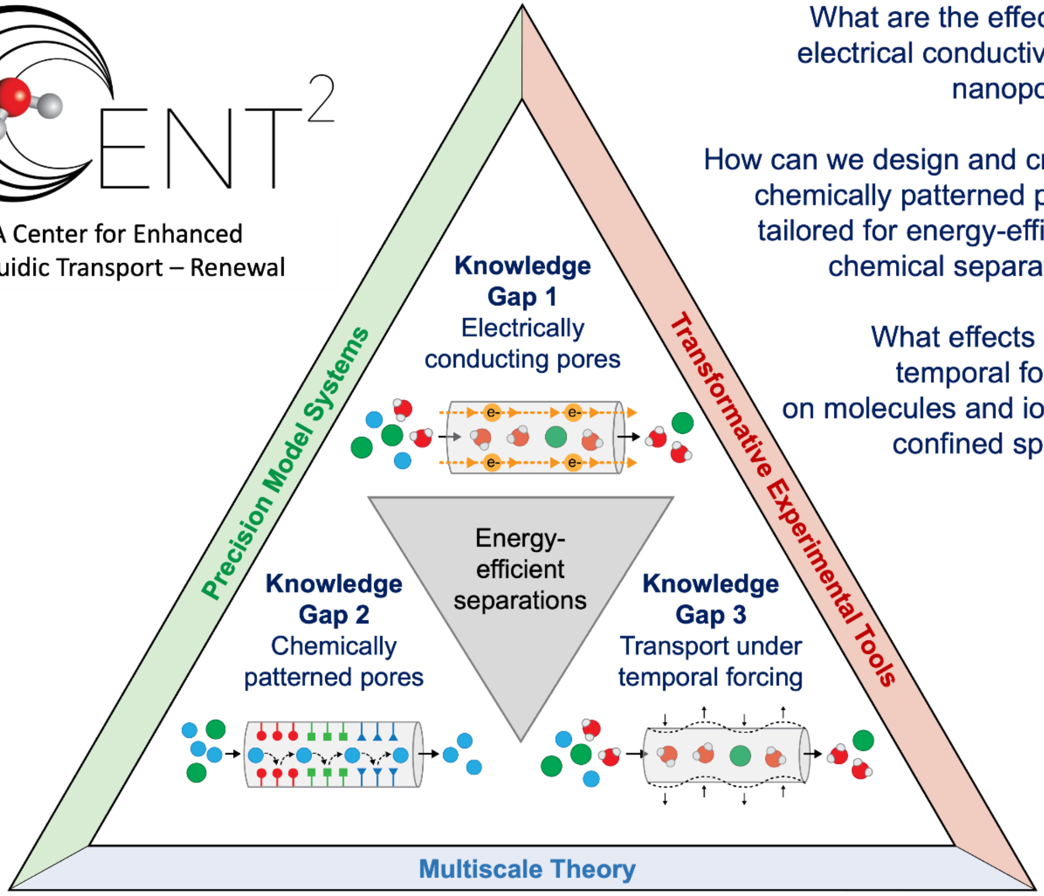
Center for Enhanced Nanofluidic Transport Phase 2 (CENT2)

Michael S. Strano (Massachusetts Institute of Technology); Class: 2018-2026

MISSION: To address critical knowledge gaps in our understanding of fluidic flow and molecular transport in extremely narrow pores. CENT2 will establish the scientific foundation for transformative molecular separation technologies impacting the water-energy nexus and *Energy Earthshots*.

RESEARCH PLAN: CENT2 will apply precision model systems, transformative experimental tools, and predictive multiscale theories to understand fluid flow and molecular transport in single-digit nanopores, to identify conditions for enhanced flow under extreme confinement, to unravel structure of solid/liquid interfaces, and to uncover new mechanisms that deliver unprecedented molecular selectivity.

EFRC: A Center for Enhanced Nanofluidic Transport – Renewal



What are the effects of electrical conductivity in nanopores?

How can we design and create chemically patterned pores tailored for energy-efficient chemical separation?

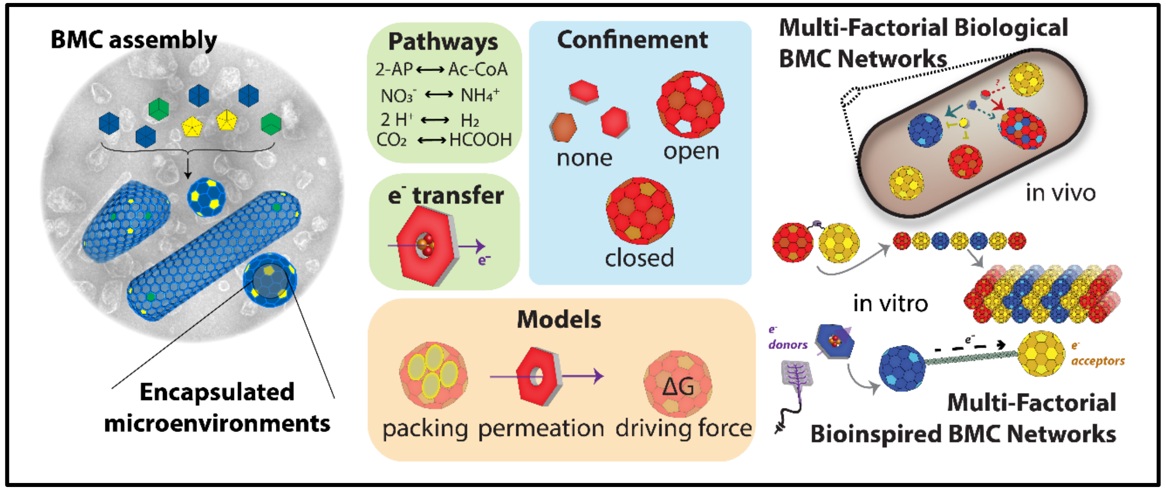
What effects have temporal forcing on molecules and ions in confined space?

cent.mit.edu

The Center for Catalysis in Biomimetic Confinement (CCBC)

Cheryl Kerfeld (Michigan State University); Class: 2022-2026

MISSION: To understand the means by which nature spatially organizes catalysis across scales using compartmentalization within selectively permeable protein-based membranes, and to use these principles to develop a modular platform for spatially organizing catalysis.



http://ccbc-efc.org/

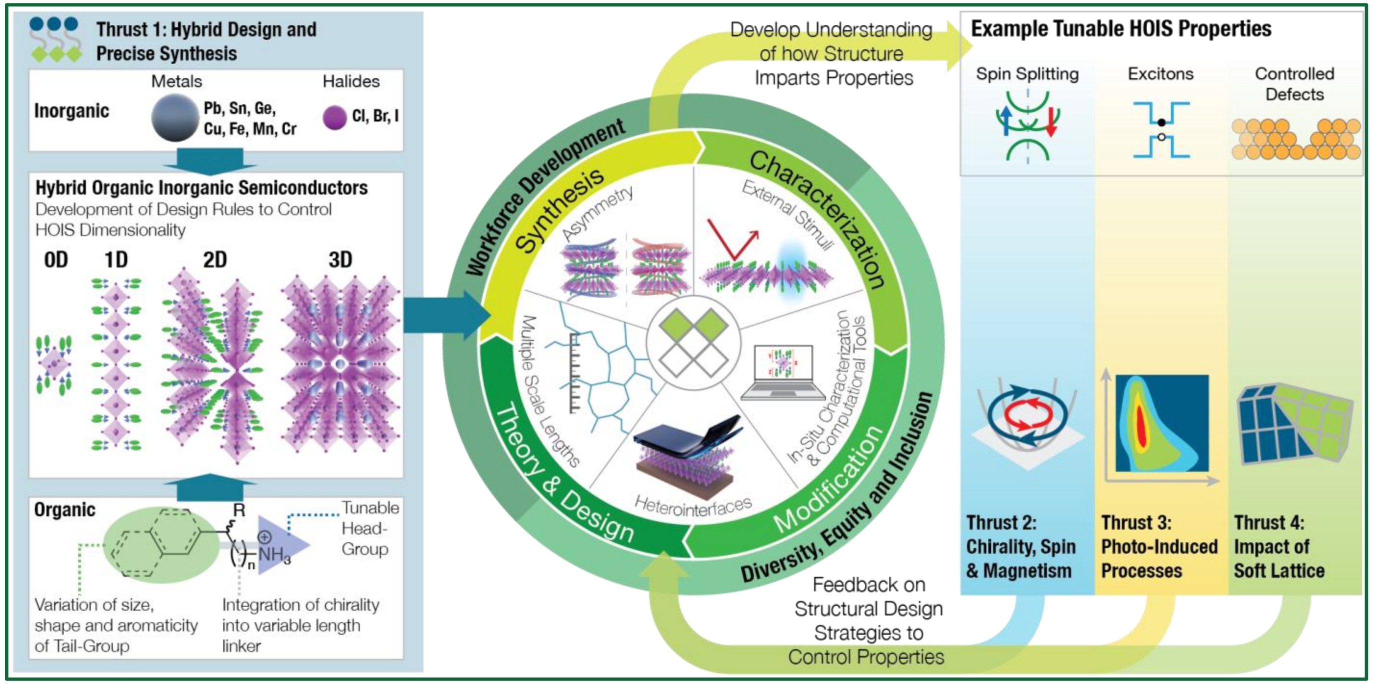
RESEARCH PLAN

The CCBC team aims to acquire a fundamental understanding of how multi-step reaction pathways are confined within and optimized by selectively permeable protein-based shells of Bacterial Microcompartments (BMCs). We will apply this knowledge to establish BMC shell proteins as building blocks that can be used for confined, hierarchically-ordered biological and synthetic multi-step catalysis for reactions that can help address global challenges related to energy and the environment.

Center for Hybrid Organic Inorganic Semiconductors for Energy (CHOISE)

Matthew C. Beard (National Renewable Energy Laboratory); Class: 2018-2026

MISSION: to demonstrate *unprecedented* control over spin, charge, phonon and light properties through synthesis and characterization of crystalline Hybrid Organic Inorganic Systems, their interfaces and heterostructures.



www.choise-efrc.org

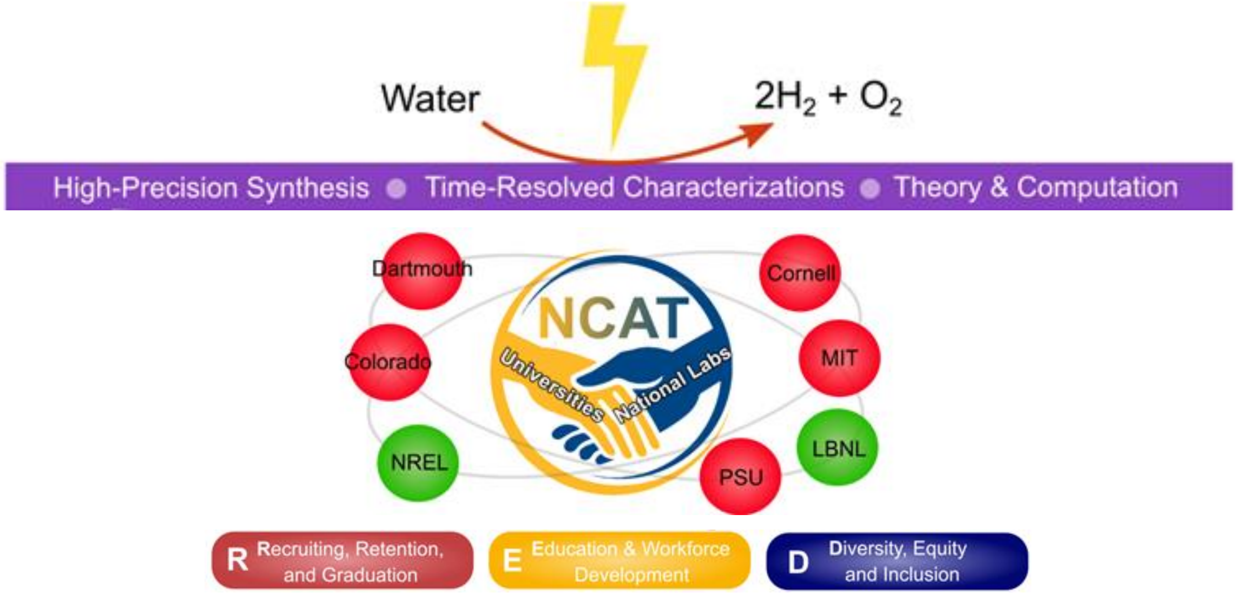
RESEARCH PLAN

We will employ the full flexibility of organic and inorganic chemistry to design and demonstrate HOIS with unique and controllable spin, electronic, and optical properties. Key structural parameters will include metal selection, halide/psuedohalide choice, overall stoichiometry, and organic cation choice.

Center for Electrochemical Dynamics and Reactions on Surfaces (CEDARS)

Dhananjay Kumar (North Carolina A & T State University); Class: 2022-2026

MISSION: To reveal the formation of the transient intermediates of oxygen evolution reaction and hydrogen evolution reaction and how the catalyst evolves before, during, and after catalysis.



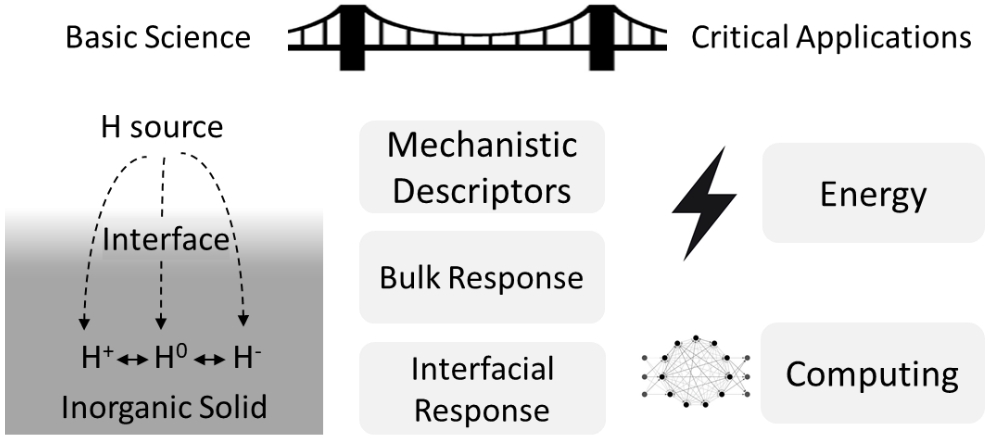
RESEARCH PLAN

CEDARS tracks the electron and proton transfer process and surface bond formation and dissociation during the hydrogen production from water splitting. CEDARS integrates high-precision materials growth with studies of the intermediates by multi-modal scattering and spectroscopy approaches, and first-principles modeling. CEDARS is multidisciplinary in nature. Its plan interweaves across disciplines, from materials, chemical, to computational sciences.

Hydrogen in Energy and Information Sciences (HEISs)

Sossina M. Haile (Northwestern University); Class: 2022-2026

MISSION: To advance the fundamental understanding and discovery of multihued hydrogen *transport* in inorganic solids of earth-abundant elements, and of its *transfer* along and across interfaces within such materials, where 'hydrogen' includes all charge states of the element: H^+ (proton), H^0 (atom), and H^- (hydride ion).



https://heiss.northwestern.edu/

RESEARCH PLAN

Leveraging the interdisciplinary expertise of the team, which spans from chemistry to materials science, and applied physics to nuclear engineering, HEISs undertakes comprehensive studies to assess hydrogen (H^+, H^0, and H^-) transport through **bulk** materials, across and along solid-solid **interfaces**, and incorporation at gas-solid **surfaces**. HEISs exploits **novel stimuli** - light, stress, and extreme electric field - and **engineered defects** – in many cases resulting from these stimuli – as routes to manipulate and enhance hydrogen dynamics.

U.S. DEPARTMENT OF ENERGY | Office of Science

Center for Bio-Inspired Energy Science (CBES)

Samuel I. Stupp (Northwestern University); Class: 2009-2024

MISSION: To develop the next frontier in soft materials relevant to energy challenges by designing structures that emulate functions we see in biological systems. CBES tackles the challenge of encoding synthetic soft materials with the ability to transduce energy forms and move autonomously in ways that are characteristic of "living matter".

https://cbes.northwestern.edu

RESEARCH PLAN

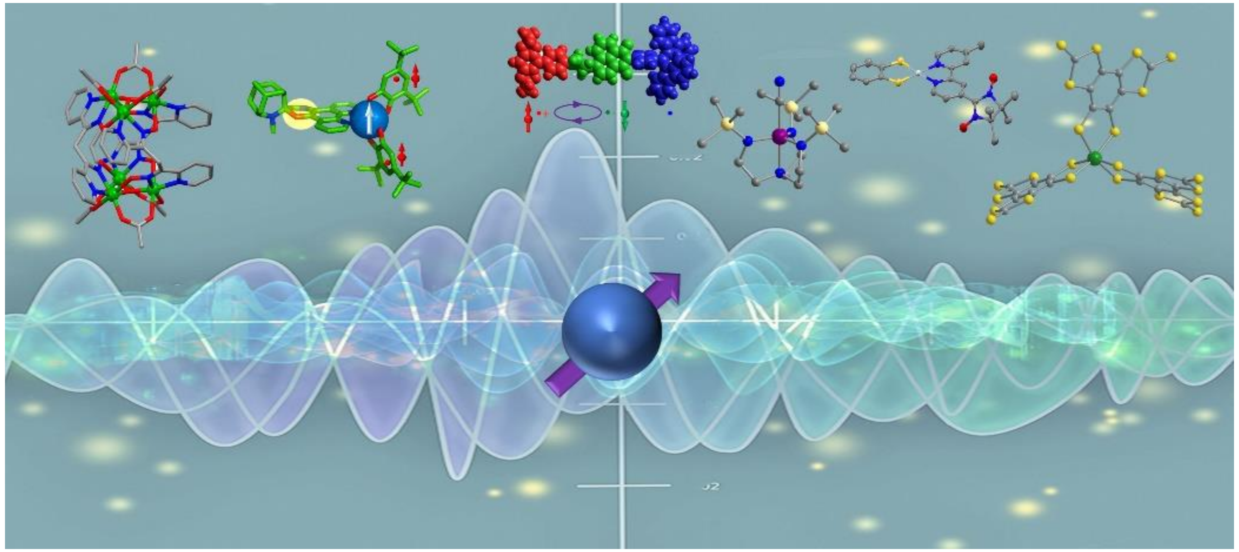
The main goals are to develop new opportunities around the concepts of "robotic soft matter", denoting the ability to rapidly perform mechanical, optical, or chemical tasks with only small inputs of energy, and "photosynthetic matter", which requires systems structured holistically to enable efficient chemical production using visible light. We approach these enormous bio-inspired challenges through bottom-up chemical design and synthesis combined with top-down engineering strategies, computation, and theory.

Center for Molecular Quantum Transduction (CMQT)

Michael R. Wasielewski, Director (Northwestern); Class: 2020-2024

MISSION: To develop the fundamental scientific understanding needed to carry out quantum transduction through a bottom-up synthetic approach which imparts atomistic precision to quantum systems.

https://isen.northwestern.edu/cmqt



RESEARCH PLAN

- **CMQT** explores coherent coupling of light, spins, and charges at the ensemble and single-molecule levels.
- **CMQT** probes quantum transduction within distributed molecular quantum systems, which bridge the length scale of single molecules with those of state-of-the-art solid-state systems.
- **CMQT** uses the interaction of light and molecular degrees of freedom to achieve quantum transduction in scalable quantum systems.

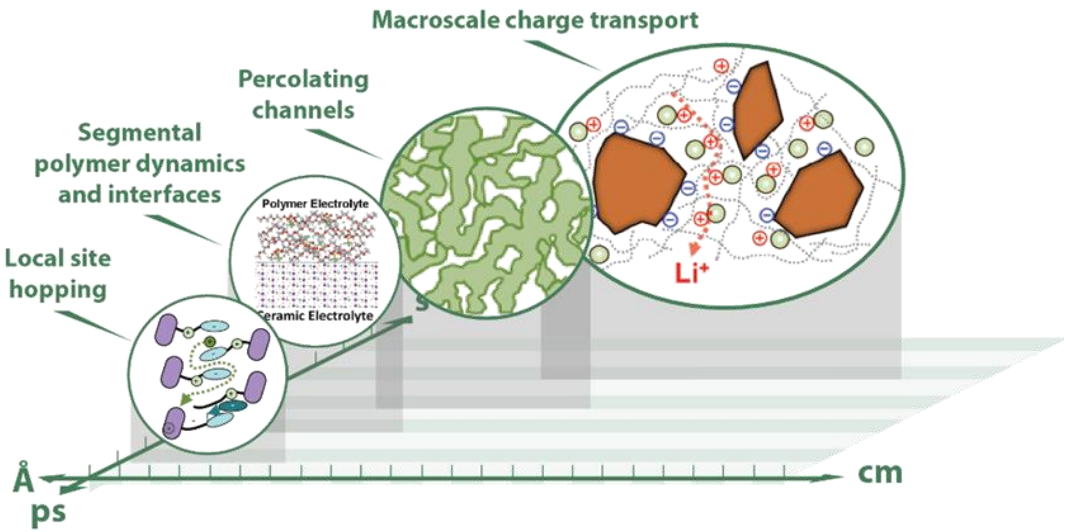
CMQT CENTER FOR MOLECULAR QUANTUM TRANSDUCTION

Northwestern
Cornell University
IOWA
THE OHIO STATE UNIVERSITY
UC San Diego
PRINCETON UNIVERSITY
Massachusetts Institute of Technology
Berkeley UNIVERSITY OF CALIFORNIA
WISCONSIN UNIVERSITY OF WISCONSIN-MADISON

Fast and Cooperative Ion Transport in Polymer Based Materials (FaCT)

Valentino R. Cooper (Oak Ridge National Laboratory); Class: 2022-2026

MISSION: To understand and control fast, correlated ion and proton transport at multiple length and time scales in polymer-based electrolytes.



https://www.ornl.gov/project/fast-and-cooperative-ion-transport-polymer-based-electrolytes-fact

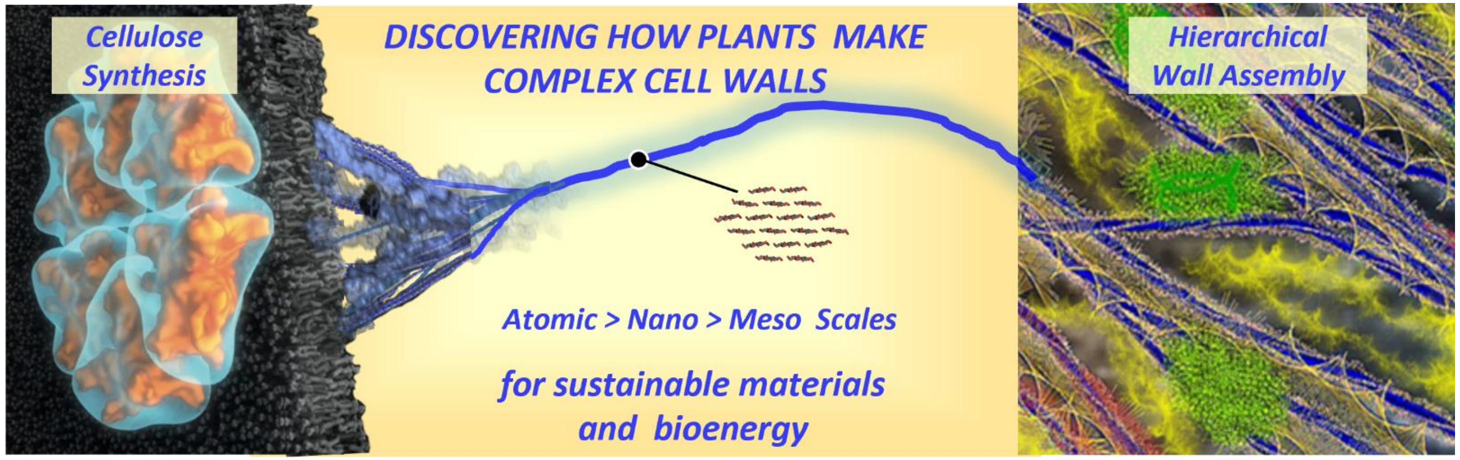
RESEARCH PLAN

FaCT seeks to examine the scientific bottlenecks limiting conductivity in polymers. The center will build a predictive, data-driven, physics-based mechanistic model of ion and proton transport in polymers and polymer-ceramic composites to enable the targeted design of next-generation energy storage and conversion materials, such as lithium ion batteries and fuel cells.

Center for Lignocellulose Structure and Formation (CLSF)

Daniel J. Cosgrove (The Pennsylvania State University); Class: 2009-2024

MISSION: to develop a nano- to meso-scale understanding of cellulosic cell walls, the energy-rich structural material in plants, and the physical mechanisms of wall assembly, forming the foundation for new technologies in sustainable energy and novel biomaterials.



www.lignocellulose.org

RESEARCH PLAN

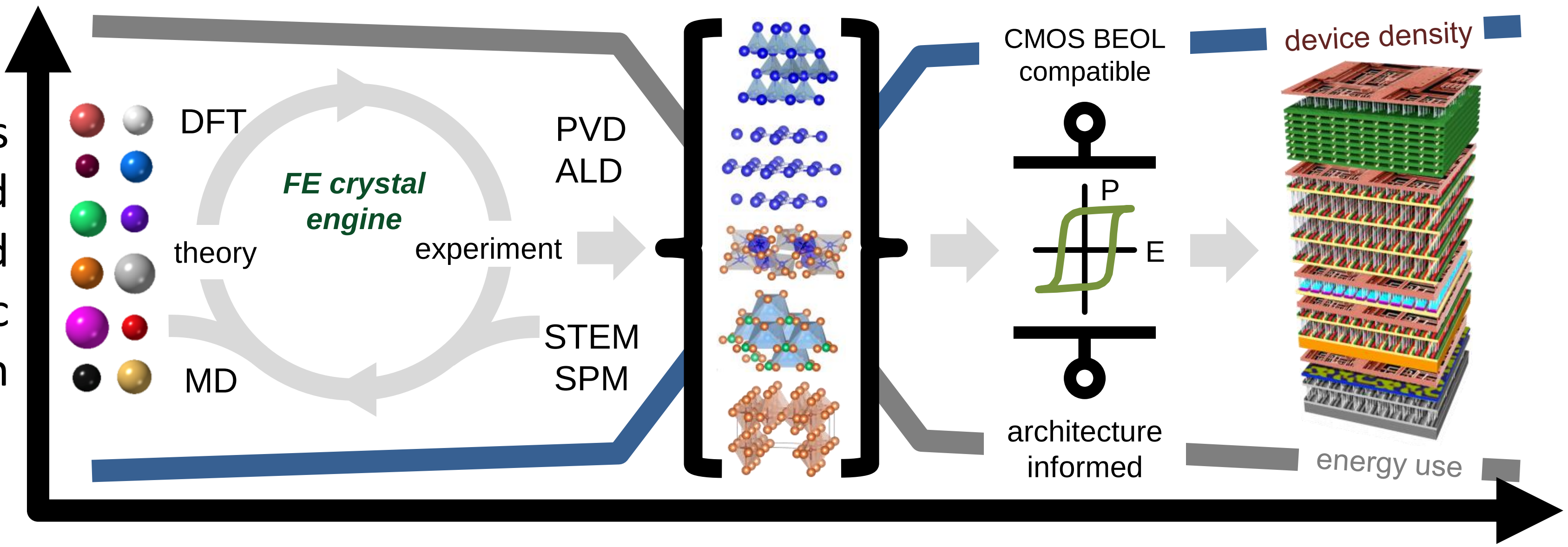
Combining cutting-edge tools of biology and physics, CLSF is elucidating (a) the nano-machinery that transforms simple sugars into cellulose microfibrils and (b) the physical processes by which cellulose interacts with matrix polysaccharides and lignin to produce hierarchically-ordered cell walls with diverse physical, chemical and material properties.

Center for 3D Ferroelectric Microelectronics (3DFeM)

Susan Trolier-McKinstry (The Pennsylvania State University); Class: 2020-2024

MISSION: Ferroelectric materials and devices that can be integrated reliably will be co-designed and densely interconnected with logic to enable low-power, 3D non-von Neumann computation.

https://3dfem.psu.edu/



RESEARCH PLAN

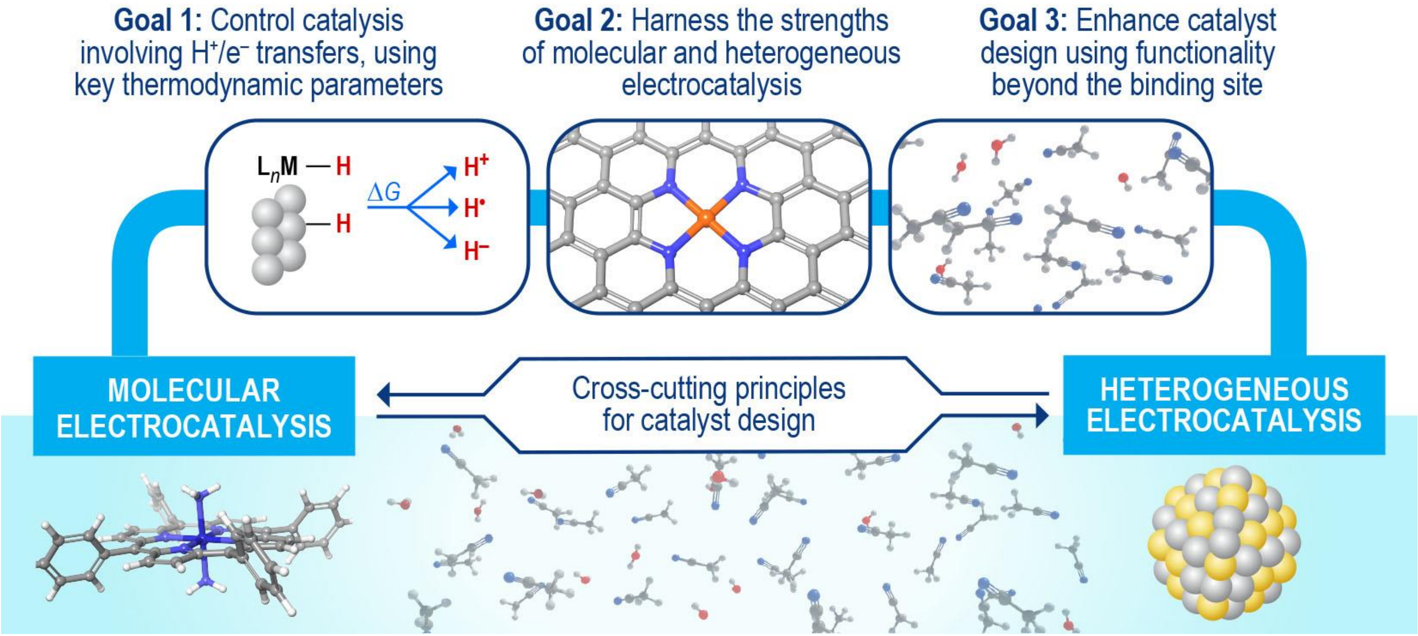
3DFeM will: (i) explore the fundamental mechanisms for emergence of ferroelectricity in new host crystal structures, (ii) tailor the coercive voltages through engineering emergent nanoscale inhomogeneity in scaled ultra-thin films, (iii) understand growth and defect dynamics in ferroelectric materials deposited with ancillary electronics at low temperatures at wafer scale, (iv) characterize materials at previously inaccessible time and length scales, and (v) demonstrate transition from materials synthesis to device functionality.

Sandia National Laboratories | Oak Ridge National Laboratory | Penn University of Pennsylvania | RIT | Georgia Tech | PennState | Purdue University | University of Virginia | Carnegie Mellon University | 3D FeM

Center for Molecular Electrocatalysis (CME)

Morris Bullock (Pacific Northwest National Laboratory); Class: 2009-2024

MISSION: To establish cross-cutting principles that facilitate catalyst design for interconversion of electrical and chemical energy, across molecular and heterogeneous catalysis.



https://efrc.pnnl.gov/cme/

RESEARCH PLAN

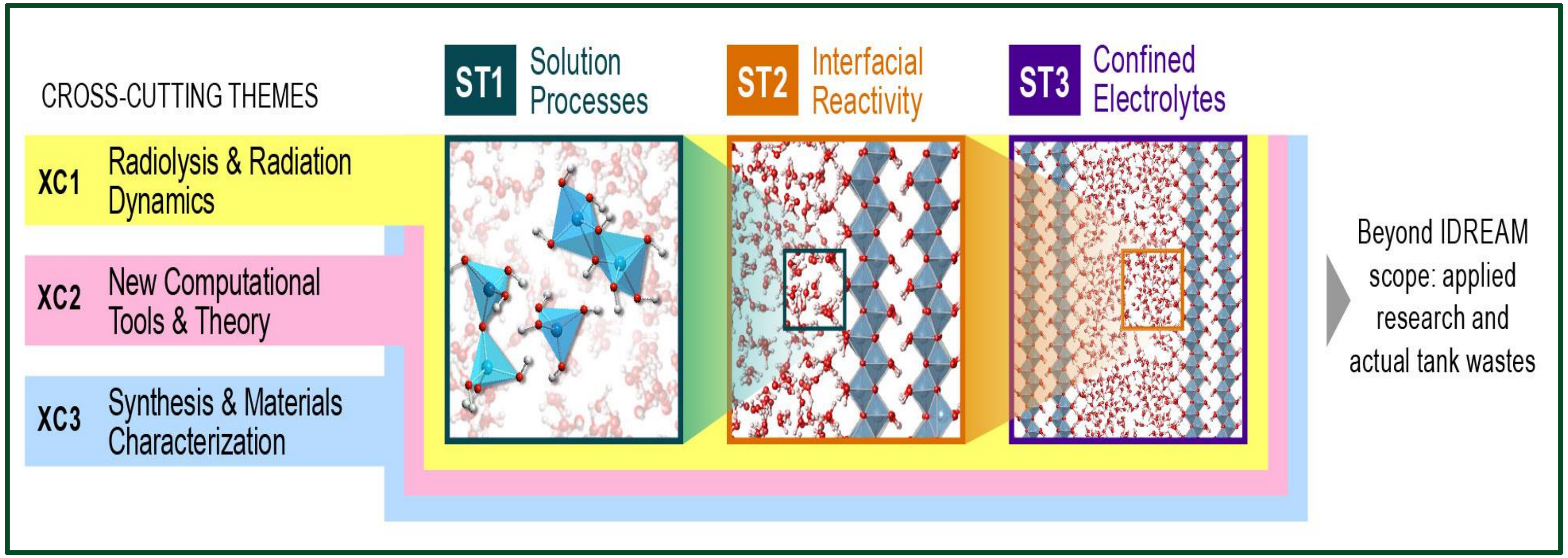
CME targets fundamental discoveries in the efficient interconversion of electrical and chemical energy through design of catalysts through a framework of proton-coupled electron transfer, bridging molecular and interfacial approaches to electrocatalysis, and harnessing the extended catalyst environment.

Interfacial Dynamics in Radioactive Environments and Materials (IDREAM)

Carolyn Pearce (Pacific Northwest National Laboratory); Class: 2016-2024

MISSION: To master fundamental chemical phenomena and interfacial reactivity in complex environments characterized by extremes in alkalinity, low-water activity, and ionizing radiation.

https://efrc.pnnl.gov/idream



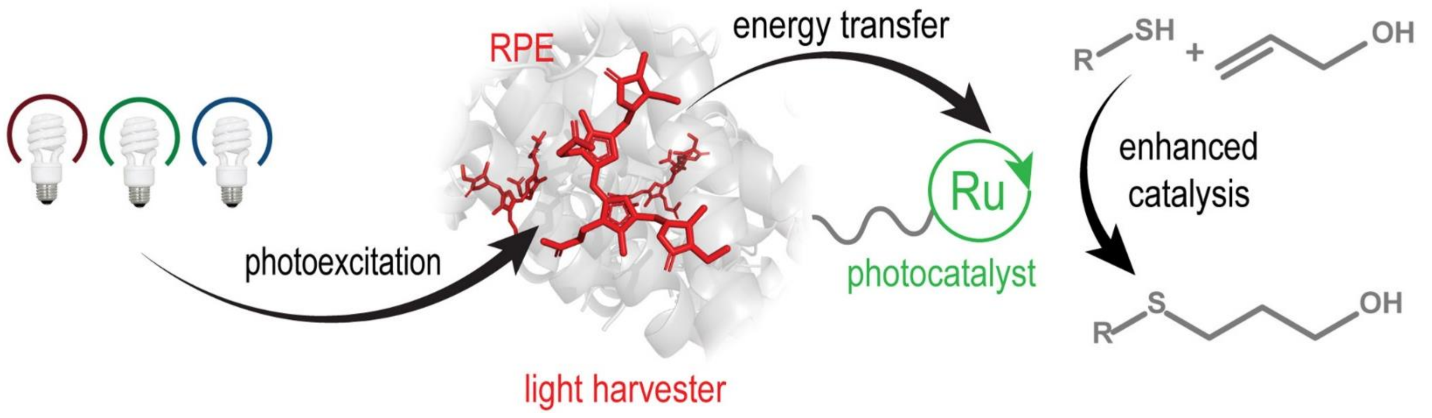
RESEARCH PLAN

IDREAM research leads to discoveries of chemical, physical, and radiolytic processes that occur in complex highly alkaline radioactive waste at DOE nuclear legacy sites. Our integrated experiments and computational modeling span atomic to macroscopic length scales of solution speciation, interfacial reactivity, and confined electrolytes, and temporal scales from sub-picoseconds to long-lived collective phenomena. Fundamental research within IDREAM enables improved technologies to process and stabilize the radioactive waste.

Bioinspired Light-Escalated Chemistry (BioLEC)

Gregory Scholes (Princeton University); Class: 2018-2026

MISSION: Inspired by nature, BioLEC uses light harvesting and advances in solar photochemistry to enable unprecedented chemical reactions that generate useful products from abundant feedstocks and waste.



www.biolec.princeton.edu

Figure reused from P. T. Cesana *et al.*, *Chem* **2022**, *8(1)*, 5, ©2022, with permission from Elsevier

RESEARCH PLAN

We aim to reduce the energy costs of chemical manufacturing by finding ways to replace fossil fuels as both energy source and starting materials. We tackle this by developing photochemistry that enables new routes for synthesizing chemical feedstocks using only light for energy; looking to nature: discovering, synthesizing and studying photoenzymes that enable enhanced catalysis; using bioinspired tactics to improve photocatalysis; and informing the design of new and improved photocatalysts by elucidating photocatalysis mechanisms.

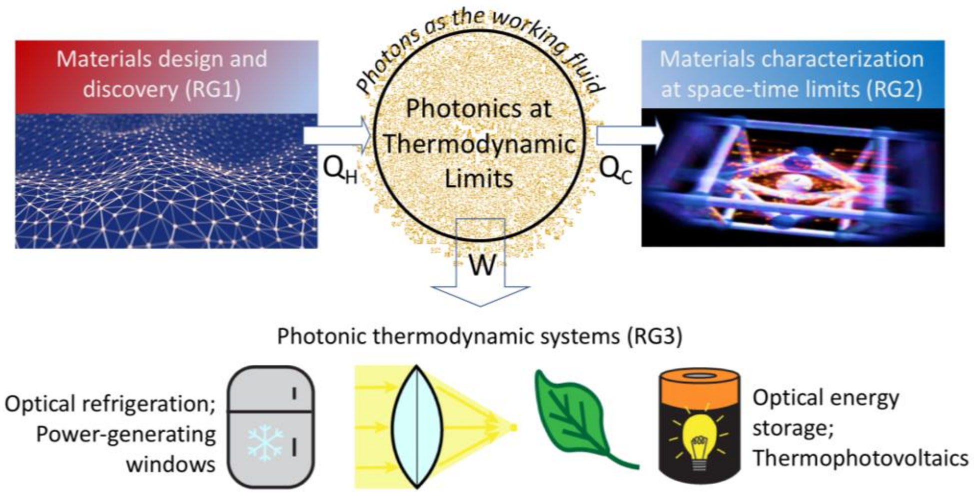
U.S. DEPARTMENT OF ENERGY | Office of Science

bioLEC

Photonics at Thermodynamic Limits (PTL)

Shanhui Fan (Stanford); Class: 2018-2024

MISSION: To achieve light-driven energy and information conversion systems that operate at thermodynamic limits by understanding and controlling the flow of photons, electrons, ions, and phonons in atomically-architectured materials.



ptl.stanford.edu

RESEARCH PLAN

- Develop new hierarchical materials, suggested by theoretical insights and synthesized with atomic precision, that perform photonic operations at thermodynamic limits.
- Develop new theoretical methods and new characterization tools, that accurately describe optically excited states and dynamic optical processes from the picometer and femtosecond scales to the system-level
- Develop a set of photonic thermodynamic cycles - such as optical refrigeration, thermophotovoltaics, and reversible computing systems - that use light as the working fluid and perform work with an efficiency approaching the Carnot efficiency

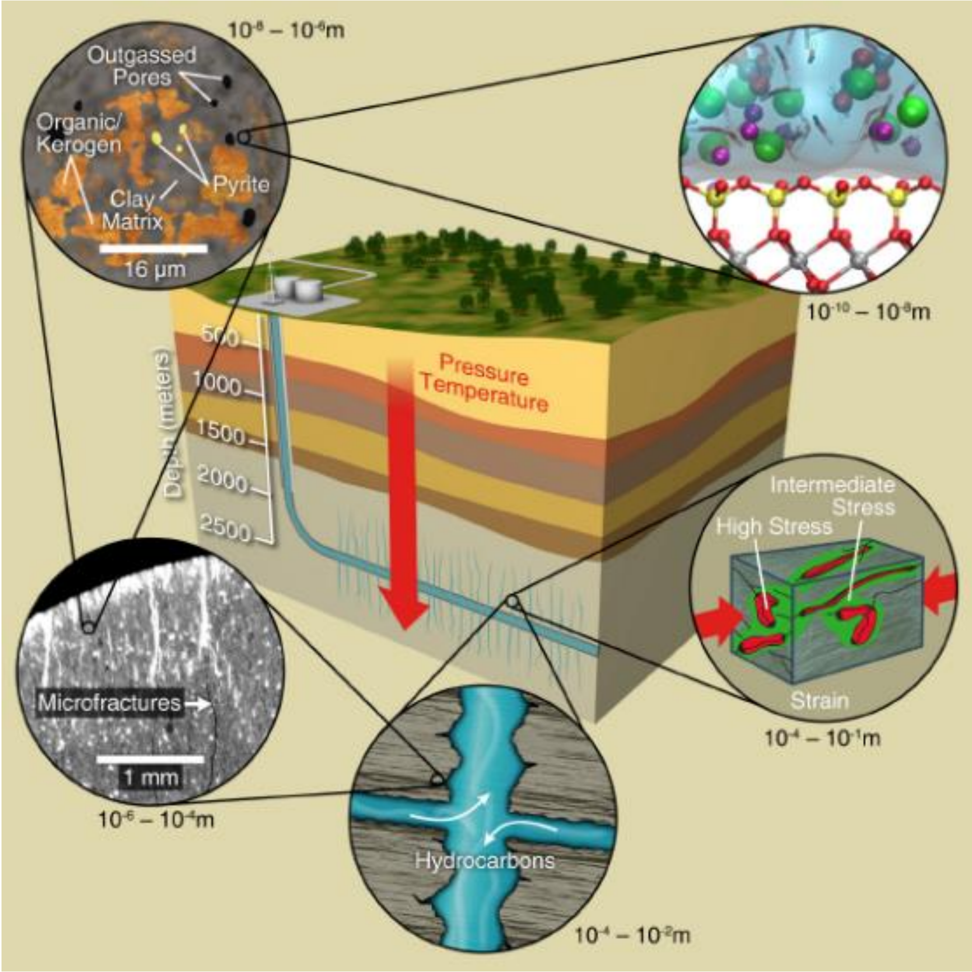
Center for Mechanistic Control of Unconventional Formations (CMC-UF)

Anthony R. Kovscek (Stanford University); Class: 2022-2024

MISSION: to garner cross-cutting geoscience knowledge to achieve mechanistic control over physical and geochemical processes in extreme geological environments collectively referred to as unconventional formations.

RESEARCH PLAN

The challenges presented by carbon management, large-scale energy storage, and improved natural gas production all require fundamental mechanistic understanding of unconventional formations, seals for storage and shales for natural gas production. With mechanistic understanding comes the potential ability to achieve control over the processes occurring in unconventional formations to improve & restore seal effectiveness and decrease negative environmental outcomes of natural gas.

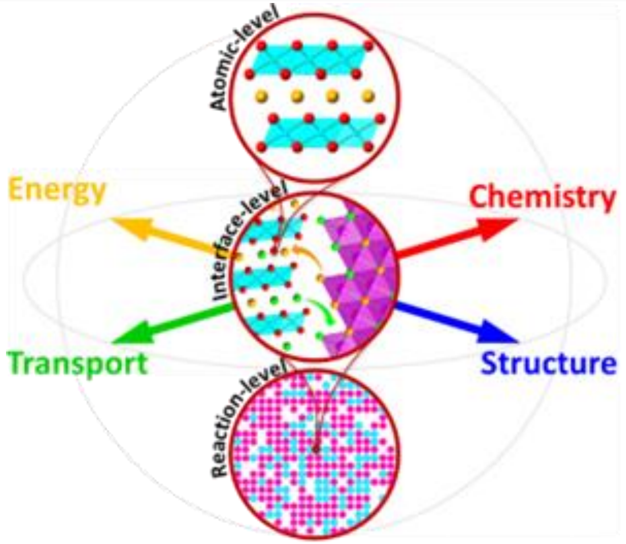


https://efrc-shale.stanford.edu/

A Next Generation Synthesis Center (GENESIS)

John Parise (Stony Brook University); Class: 2018-2024

MISSION: To elucidate how key structural and chemical transformations are governed by the flow of energy and atoms across multiple length scales, and to enable precision synthesis of targeted new materials by integrating advanced in situ diagnostics and data science tools to interrogate and predict non-equilibrium synthesis pathways.



https://www.stonybrook.edu/genesis/

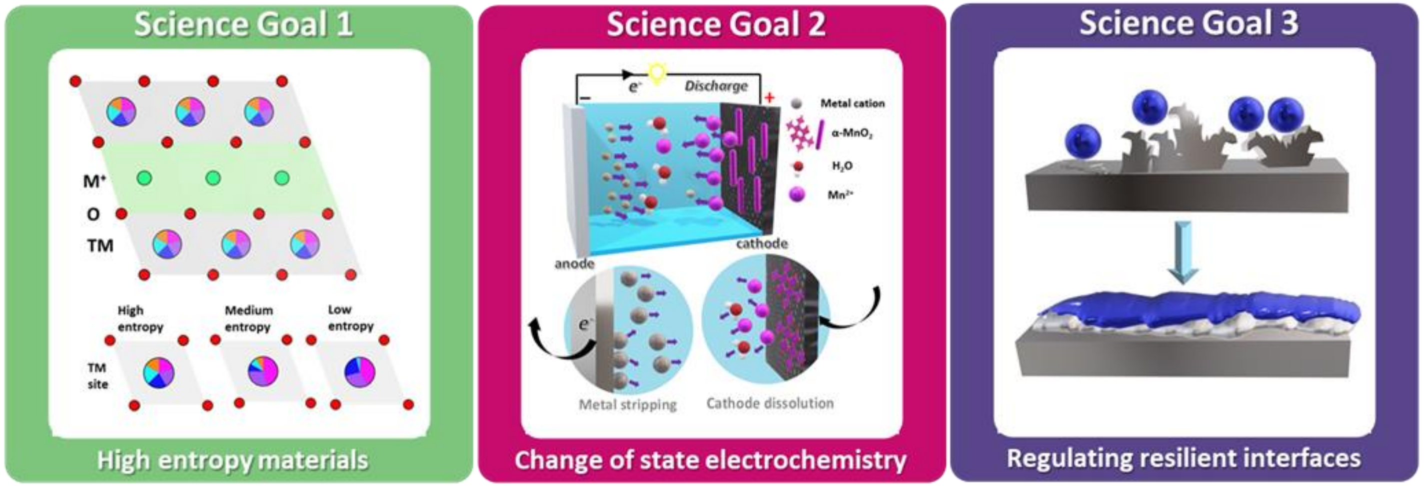
RESEARCH PLAN

Our aim is to control precise materials synthesis at 1) the atomic scale, requiring control of atomic configurations, composition, structural defects and impurities, which are governed by the relative mobilities of species and the relative energetics of competing structural phases, and 2) at the mesoscale (interfacial, particle- and reaction-scales), by controlling collective effects, including chemical microenvironments, relative kinetics in transport-limited reaction architectures, heterogeneity, compositional gradients, and microstructure.

Center for Mesoscale Transport Properties (m2m#S)

Amy Marschilok (Stony Brook University); Class: 2014-2026

MISSION: To understand and harness disorder and entropy to build the science foundation for new design spaces that enable sustainable, long cycle life electrochemical energy storage.



https://www.stonybrook.edu/commcms/m2m/

RESEARCH PLAN

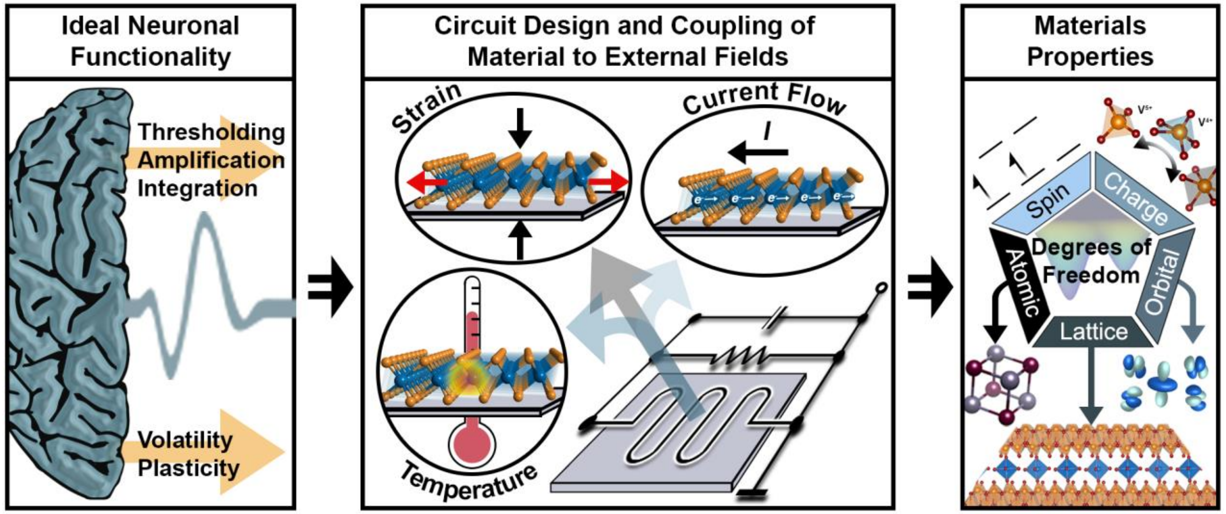
The Center will integrate synthesis, characterization, theory, modeling and electrochemistry to achieve its science goals of exploring new earth abundant electroactive materials, understanding and controlling electrochemical processes in sustainable systems, and favorably manipulating interfaces.

Stony Brook University · Brookhaven National Laboratory · Columbia University in the City of New York · Cornell University · Berkeley Lab Lawrence Berkeley National Laboratory · Lehigh University · Texas The University of Texas at Austin · Xavier University of Louisiana · m2m#S molecular to mesoscale

Reconfigurable Electronic Materials Inspired by Nonlinear Neuron Dynamics (REMIND)

R. Stanley Williams (Texas A&M Engineering Experiment Station); Class: 2022-2026

MISSION: to establish foundational scientific knowledge underpinning the function of massively reconfigurable computing architectures that approach fundamental limits of energy efficiency and speed, enabling real-time learning and embedded intelligence emulative of specific neuronal and synaptic functions of the human brain.



www.remind.engr.tamu.edu

RESEARCH PLAN

REMIND seeks to *flip the current computing paradigm* by blending *inverse* and *forward* design and connecting *dynamical material properties and underlying transformations* to *discover and exploit* new materials, mechanisms, and interfaces that are required to emulate specific neuronal and synaptic functions of the human brain. REMIND will uncover fundamental mechanisms and molecular/material building blocks for a new paradigm of brain-inspired computing.

remind TEES Texas A&M Engineering Experiment Station NREL Transforming ENERGY Sandia National Laboratories BERKELEY LAB

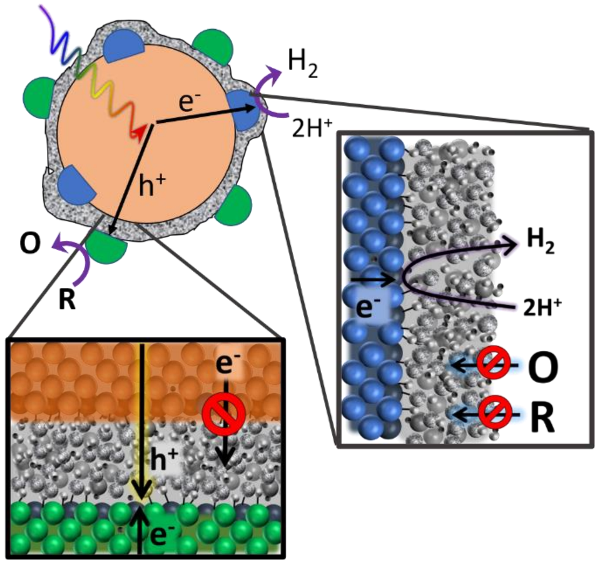
U.S. DEPARTMENT OF ENERGY Office of Science

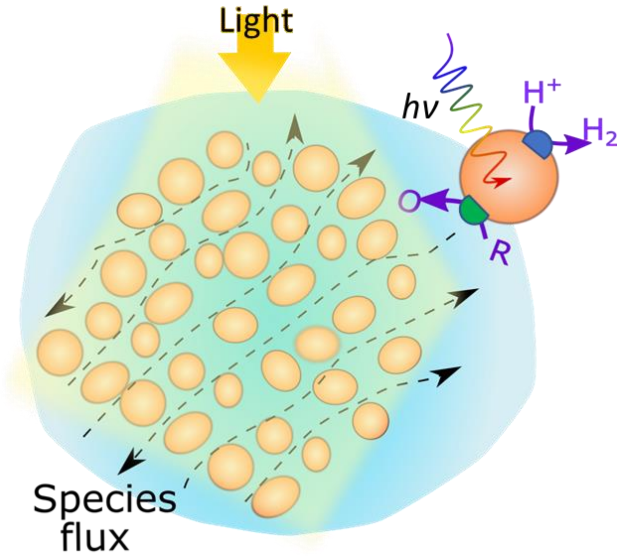
Ensembles of Photosynthetic Nanoreactors (EPN)

Shane Ardo (University of California Irvine); Class: 2022-2026

MISSION: To understand, predict, and control the activity, selectivity, and stability of solar water splitting nanoreactors in isolation and as ensembles.

https://photosynthesis.uci.edu/





RESEARCH PLAN

EPN will strive to advance the frontiers of discovery and fundamental interdisciplinary knowledge in photochemical energy conversion basic science and engineering. Research goals are to extend photocarrier lifetimes and control their dynamics during infrequent photon absorption events; enhance charge-separation yields and redox selectivity, and therefore stability, under conditions of low-flux carrier transport; and program ensembles of artificial photosystems for large solar-to-hydrogen energy conversion efficiencies.

Center for Closing the Carbon Cycle (4C)

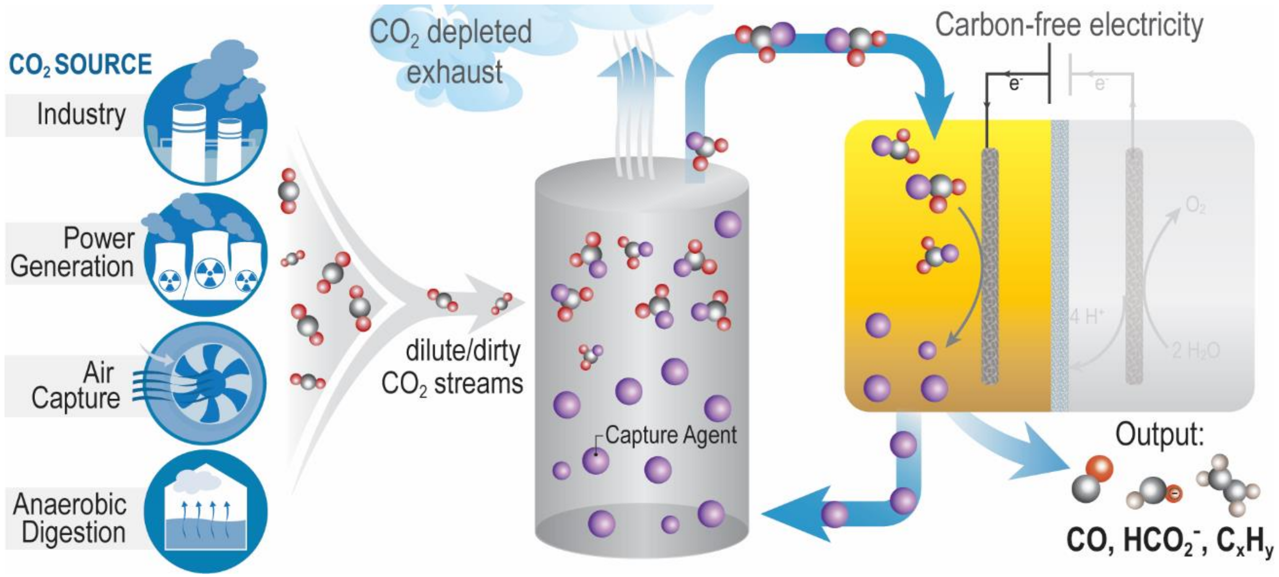
Jenny Y Yang (University of California, Irvine); Class: 2022-2026

MISSION: To advance synergistic capture and conversion of carbon dioxide (CO_2) from dilute streams into useful products through the convergent study of sorbents and catalysts.

RESEARCH PLAN

4C will advance the foundational science and define key integration parameters for synergistic CO_2 capture and conversion, or reactive capture of CO_2 (RCC). By co-designing CO_2 sorbent capture with catalysts, 4C will develop integrated RCC systems that work cooperatively to achieve higher product selectivity and overall efficiencies than current sequential approaches.

https://carbonsolution.uci.edu/about.html



UCI · Lawrence Livermore National Laboratory · Oak Ridge National Laboratory · UCLA · UC Davis · UC Merced · University of Colorado Boulder · University of Central Arkansas · Cal Poly Pomona · University of Michigan · ECSU Elizabeth City State University Founded 1891 · California Institute of Technology · Case Western Reserve University · Pacific Northwest National Laboratory

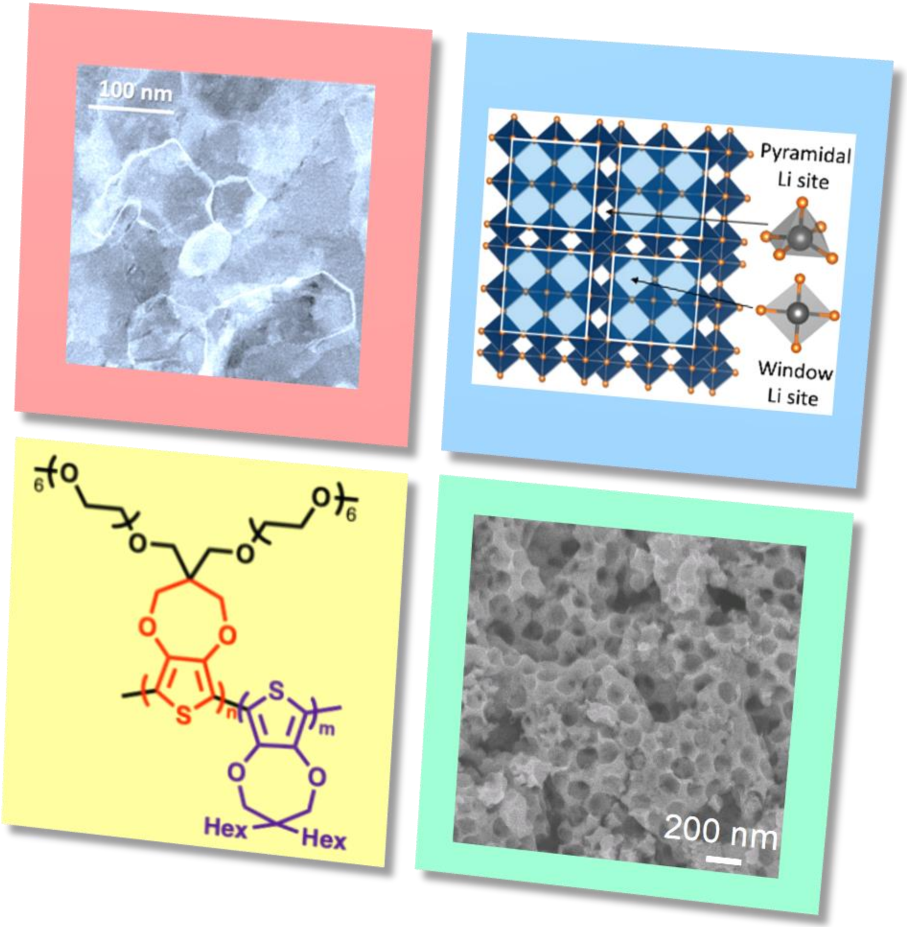
Synthetic Control Across Length-scales for Advancing Rechargeable (SCALAR)

Sarah Tolbert (UCLA); Class: 2018-2024

MISSION: To use the power of synthetic materials chemistry to design materials, interfaces, and architectures that help solve long-standing problems in electrochemical energy storage.

RESEARCH PLAN

The SCALAR center aims to take a holistic approach to the design of new functional materials that bridges the atomistic, nanometer, and macro length-scales in the quest to improve battery performance. To do this, the center will leverage molecular and solid-state synthetic methods, combined with solution phase self-assembly, to create new electrode materials that increase capacity, reduce losses, and improve reversibility in rechargeable batteries.

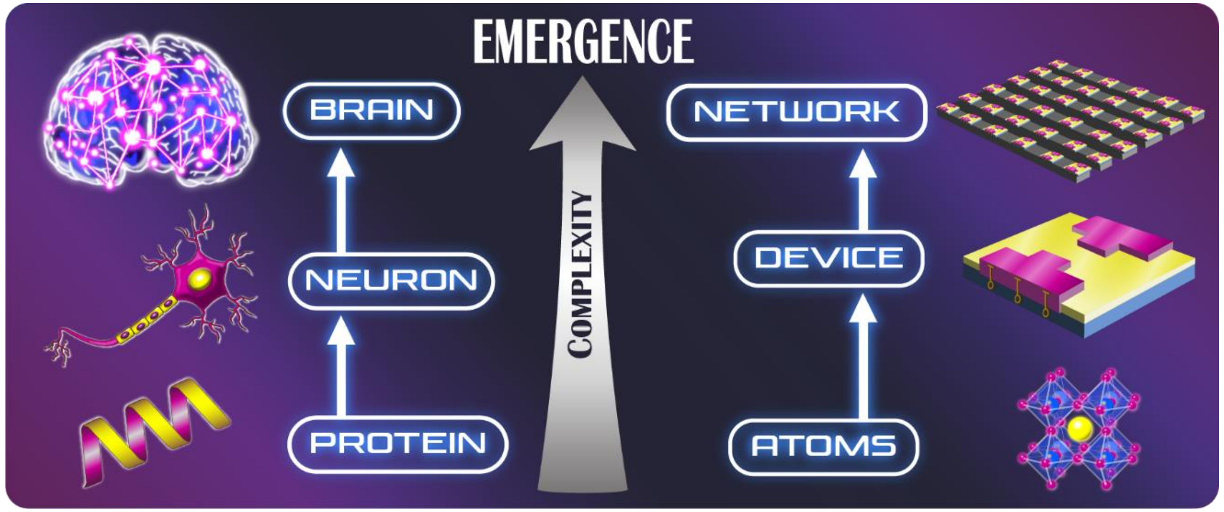


http://www.chem.ucla.edu/SCALAR

Quantum Materials for Energy-Efficient Neuromorphic Computing (Q-MEEN-C)

Ivan K. Schuller (UCSD); Class: 2018-2026

MISSION: To lay down the quantum-materials-based foundation for the development of an energy-efficient, fault-tolerant computer that is inspired and works like a brain ("neuromorphic").



https://qmeenc.ucsd.edu/

RESEARCH PLAN

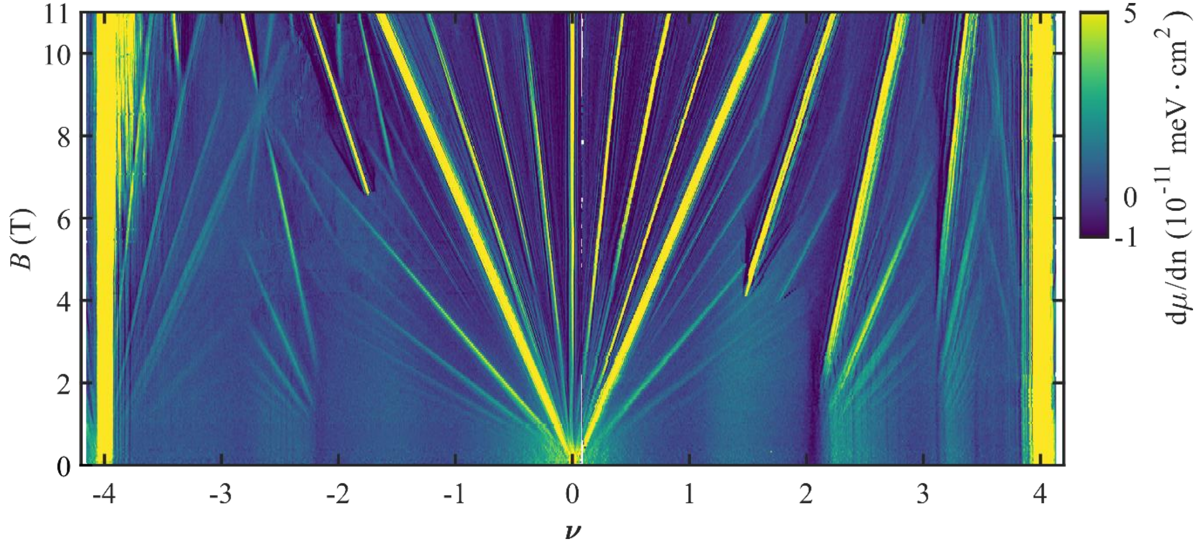
Synthesize promising new quantum materials for neuromorphic functionalities. Understand their microscopic and mesoscopic behavior due to natural and/or artificial inhomogeneities, develop novel contactless connectivity using collective or frequency selective mesoscopic coupling, and define new benchmarks for relevant materials properties and energy efficiency.

Quantum Materials for Energy Efficient Neromorphic Computing

Quantum Sensing and Quantum Materials (QSQM)

Peter Abbamonte (University of Illinois, Urbana-Champaign); Class: 2020-2024

MISSION: To develop new quantum sensing techniques and apply them to investigate relationships between the local and global properties of quantum materials that exhibit strong correlations and/or topological order.



https://iquist.illinois.edu/programs/qsqm

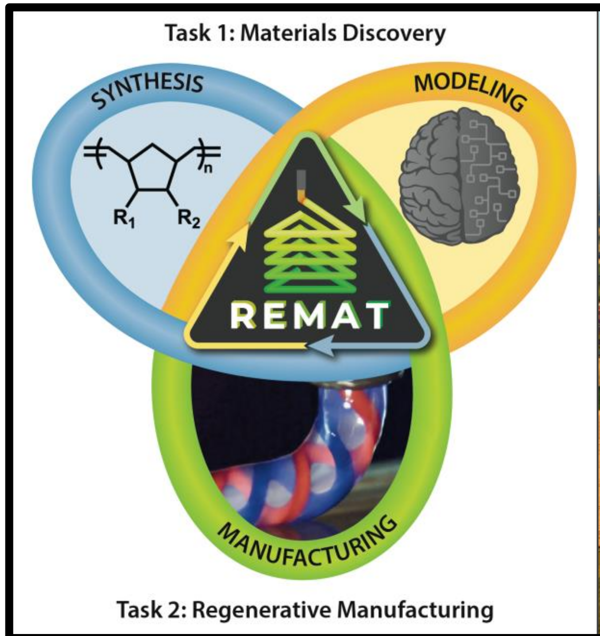
RESEARCH PLAN

QSQM is building a scanning qubit microscope to explore localized electronic states and exotic excitations in quantum materials. QSQM is also developing Einstein-Podolsky-Rosen (EPR) spectroscopy, which is a two-electron time-of-flight technique that will reveal valence band interaction effects in superconductors and determine the microscopic origin of electron-electron interactions and the degree of correlations in strange metals and topological crystalline insulators.

Regenerative Energy-Efficient Manufacturing of Thermoset Polymeric Materials (REMAT)

Nancy Sottos (University of Illinois, Urbana-Champaign); Class: 2022-2026

MISSION: To advance the science of thermochemical reaction-diffusion processes in additive and morphogenic manufacturing and accelerate a transformative, circular strategy for thermoset polymeric and composite materials with programmed end-of-life.



www.remat.edu

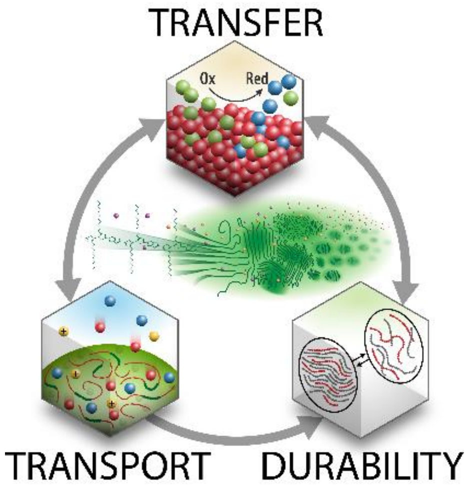
RESEARCH PLAN

The Center's goal is to discover thermoset resin formulations that enable (i) closed-loop controlled, energy-efficient additive manufacturing, (ii) nascent morphogenic manufacturing strategies, (iii) programmed end-of-life upcycling, and (iv) precise understanding of the chemistry and physics that control properties, performance, and multifunctionality for (re)use in structural materials.

Center for Soft PhotoElectroChemical Systems (SPECS)

Erin Ratcliff (University of Arizona); Class: 2022-2026

MISSION: To understand the factors controlling charge and matter transport processes in inexpensive, scalable, and durable π-conjugated polymer (plastic) materials, and to explore the factors across spatiotemporal scales that underpin emerging energy conversion technologies to influence the formation of fuels, such as H_2, from sunlight and develop new approaches to energy storage.



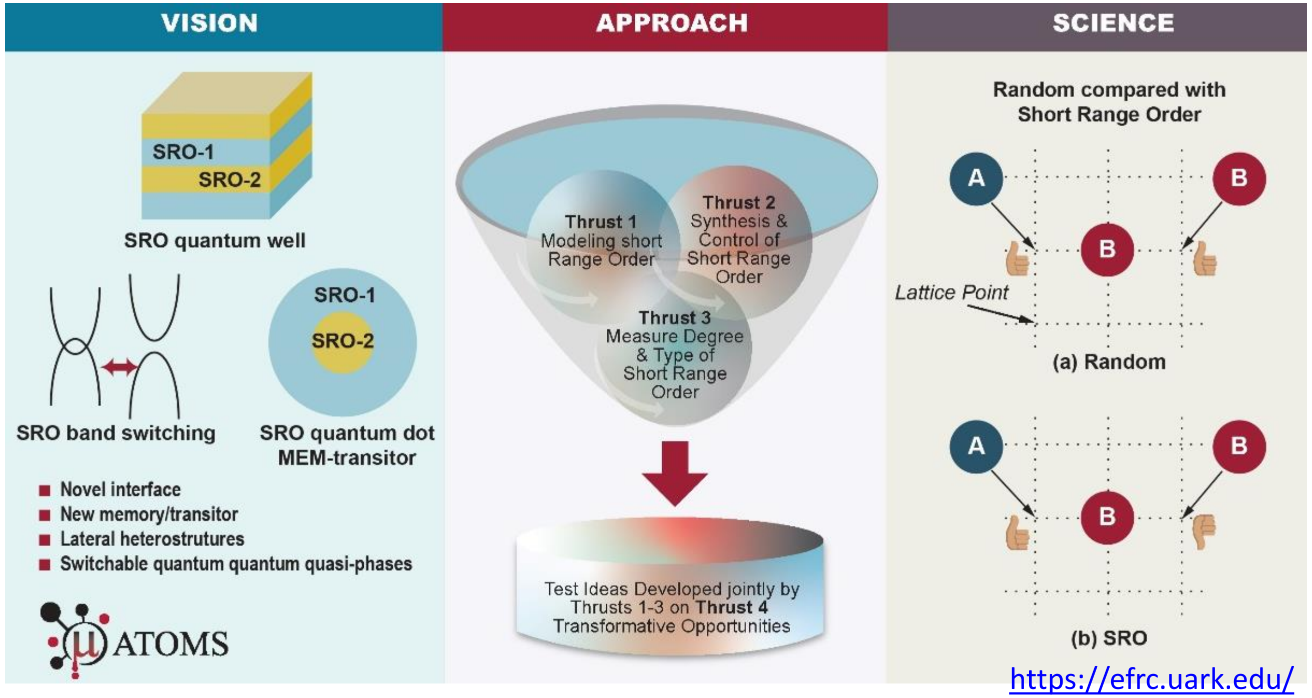
http://specs.arizona.edu/

RESEARCH PLAN

SPECS is organized around three interconnected thrusts. ***Thrust 1: Hybrid Electrical-Ionic Charge Transport*** will understand and control the complex polymer/electrolyte structures that control ion and charge transport relevant to energy conversion and energy storage processes. ***Thrust 2: Charge Transfer and Energy Cascades*** will understand and optimize polymer photocathodes for efficient charge transfers to drive fuel-forming reactions such as formation of H_2. ***Thrust 3: Durability*** focuses on creation of a molecular and material scale understanding, leading to design guidelines for creation of robust energy conversion and storage systems.

Manipulation of Atomic Ordering for Manufacturing Semiconductors (μ-ATOMS)
Shui-Qing "Fisher" Yu (University of Arkansas); Class: 2022-2026

MISSION: To discover the underlying science principles determining the ordering of atoms in semiconductor alloys.



https://efrc.uark.edu/

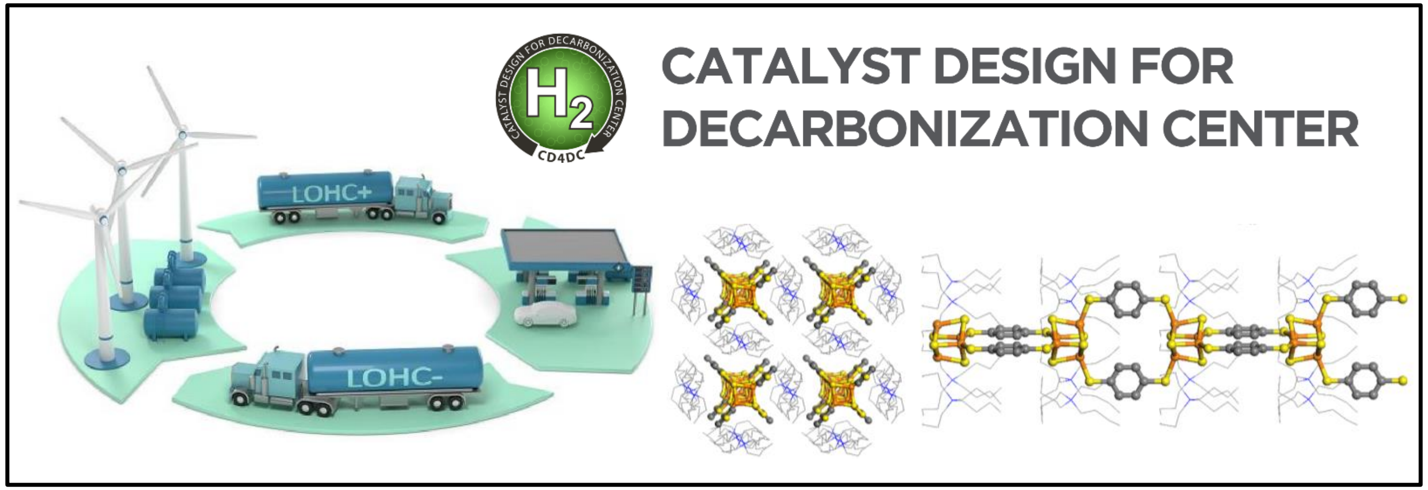
RESEARCH PLAN

μ-ATOMS will model both material and structure to guide fabrication, develop and demonstrating new synthesis tools and techniques, use a suite of new characterization tools to develop the measurement ability, and controlling atomic order in semiconductor alloys for transformative opportunities enabled by the new optical, electrical, quantum, and structure transition properties.

Catalyst Design for Decarbonization Center (CD4DC)

Laura Gagliardi (University of Chicago); Class: 2022-2026

MISSION: To discover and develop reticular metal-organic framework materials as catalysts for the decarbonization energy transition and to optimize the key catalytic reactions involved.



https://cd4dc.center.uchicago.edu/

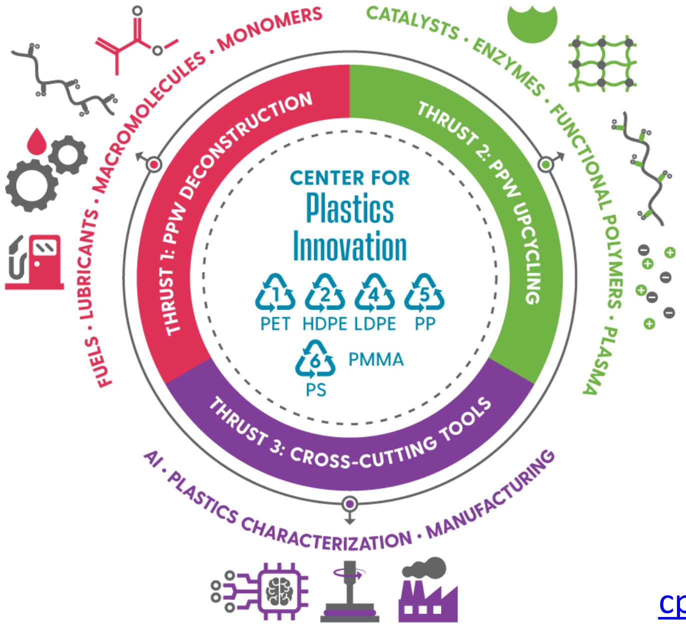
RESEARCH PLAN

CD4DC will address the essential need for alternate forms of H_2 transport and storage, via the development of methanol and liquid organic hydrogen carriers (LOHCs). CD4DC will discover new, low temperature, high activity catalysts for H_2 addition and removal, and C-C bond formation. We will link synthesis of catalytic materials, catalytic transformations and the kinetic description of the transformations, characterization of catalysts and organic species, computational modeling and active learning.

Center for Plastics Innovation (CPI)

LaShanda Korley (University of Delaware); Class: 2020-2024

MISSION: To: (1) Develop catalytic and functionalization approaches and fundamental tools applicable to the upcycling, upgrading, and recycling of real polymer plastics waste (PPW) with a strategic focus on enabling mixed-stream transformations in varied material forms (*i.e.,* solutions, melts, and surfaces); (2) Educate the future U.S. workforce for relevant industries; and (3) Enable PPW-related innovations *via* technology transfer, licensing, and start-up formation.



cpi.udel.edu

RESEARCH PLAN

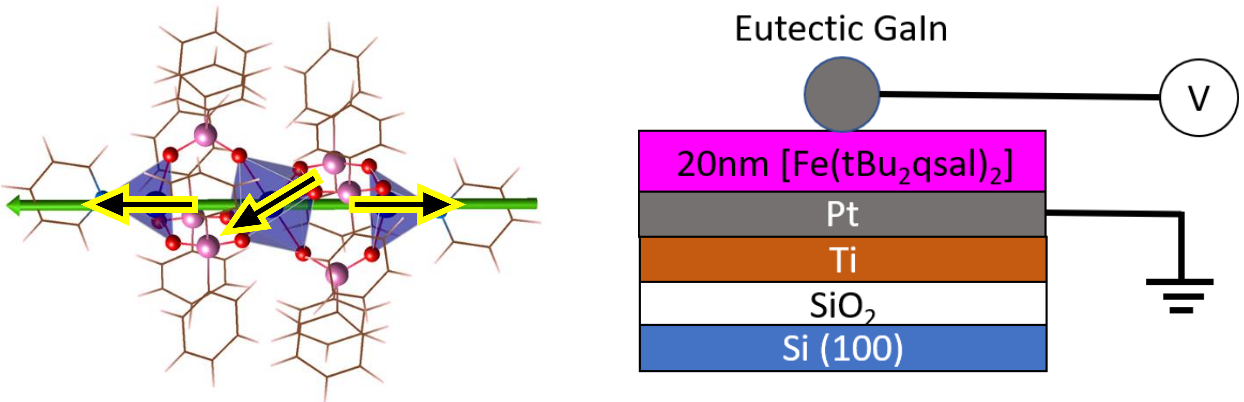
CPI will develop a comprehensive polymer plastics waste (PPW) upcycling strategy that combines fundamental discoveries in catalytic technology and chemical functionalization with innovations in polymer design and additive manufacturing – enabled by computational, data science, characterization, and systems design tools. Our vision is that these fundamental breakthroughs will enable efficient and selective processes to overcome the environmental impacts of increasing plastics waste.

EFRC for Molecular Magnetic Quantum Materials (M^2QM)

Hai-Ping Cheng (University of Florida); Class: 2018-2026

MISSION: To provide the materials physics and chemistry understanding of molecular magnetic quantum materials essential for quantum and conventional computing beyond Moore's Law, with an overarching goal of turning molecular magnets into quantum materials useful for both quantum computing and quantum current conventional devices.

From molecules to magnetics junctions



www.efrc.ufl.edu

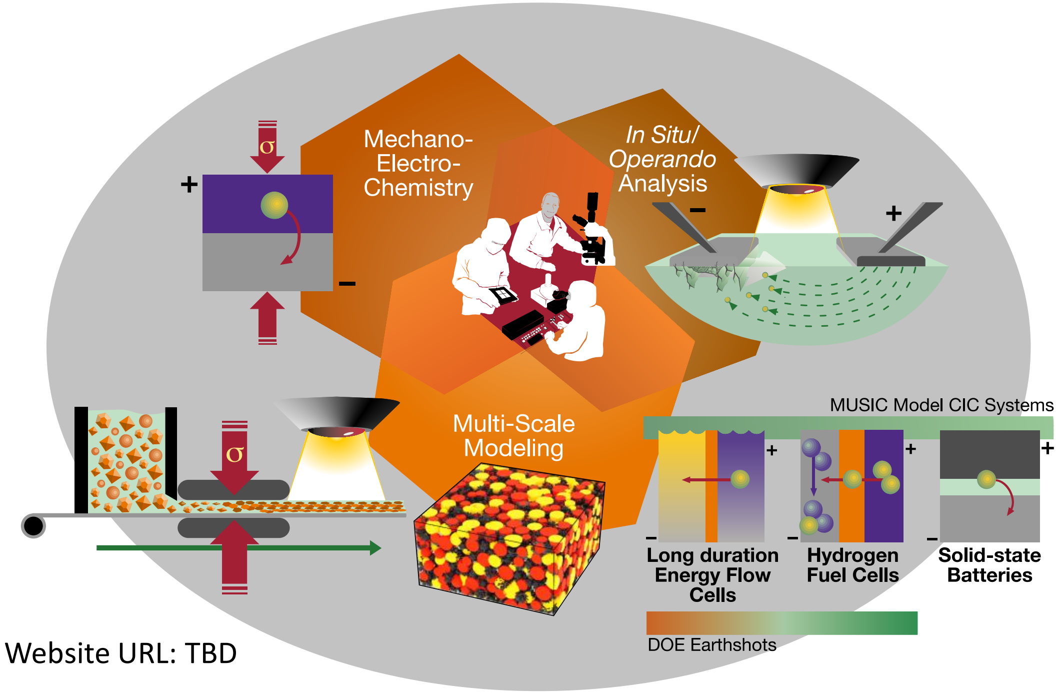
RESEARCH PLAN

From synthesis to characterization (experimentally and computationally), the central quest of the M^2QM project is to achieve such magnetic switching at molecular scale and to achieve switching and reading electronically. This would have a more profound outcome than reduction of heating. It would enable quantum computing – working with molecular states that are both one and zero and in-between. This is the shift from "bits" to "qubits". The molecular state that is critical to its magnetism is called the "spin state".

Mechano-Chemical Understanding of Solid Ion Conductors (MUSIC)

Jeff Sakamoto (University of Michigan); Class: 2022-2026

MISSION: To reveal, understand, model, and ultimately control the chemo-mechanical phenomena underlying the processing and electrochemical dynamics of ceramic ion conductors (CICs) for clean energy systems.



Website URL: TBD

RESEARCH PLAN

Thrust 1: Revealing electrochemical-mechanical coupling at CIC interfaces and interphases

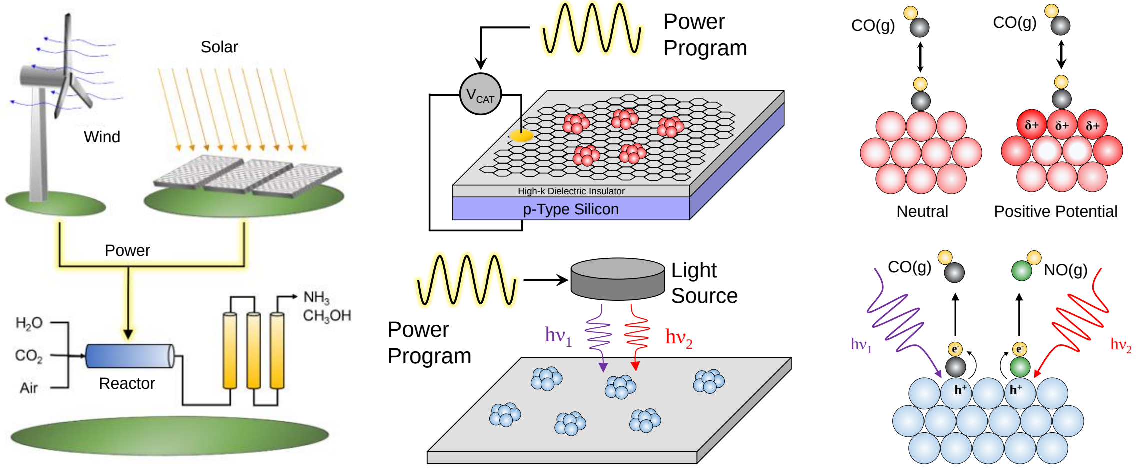
Thrust 2: Understanding material degradation pathways in CIC-based electrochemical systems

Thrust 3: Science of synthesis, processing, and manufacturing of CICs

Center for Programmable Energy Catalysis (CPEC)

Paul J. Dauenhauer (University of Minnesota); Class: 2022-2026

MISSION: To transform how catalysts control energy, and to accelerate surface reactions beyond kinetic limitations using rapid perturbations of light and charge in programmed oscillations that alter the flow of energy at the surface and control the behavior of molecules and chemistry for renewable energy storage.



www.cpec.umn.edu

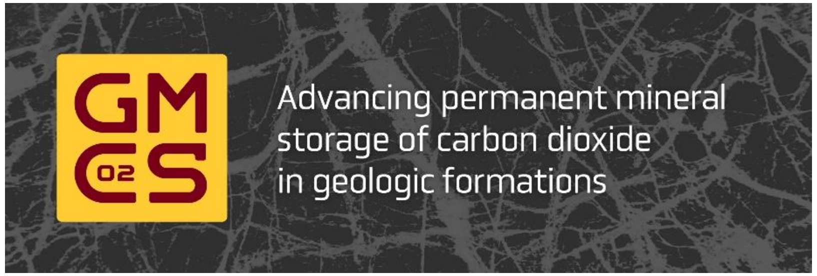
RESEARCH PLAN

CPEC aims to understand how electrons rearrange on metal and metal oxide surfaces such that they can be programmed to optimally control catalytic reactions. The power programs that temporally control the catalyst surface will be designed to promote targeted products at higher rates using a combination of modeling and experiment of two catalytic systems (dynamic photocatalysis and programmable catalytic condensers) that are designed for maximum power and oscillation frequency control with variable active surface compositions.

Geo-processes in Mineral Carbon Storage (GMCS)

Emmanuel Detournay (University of Minnesota); Class: 2022-2026

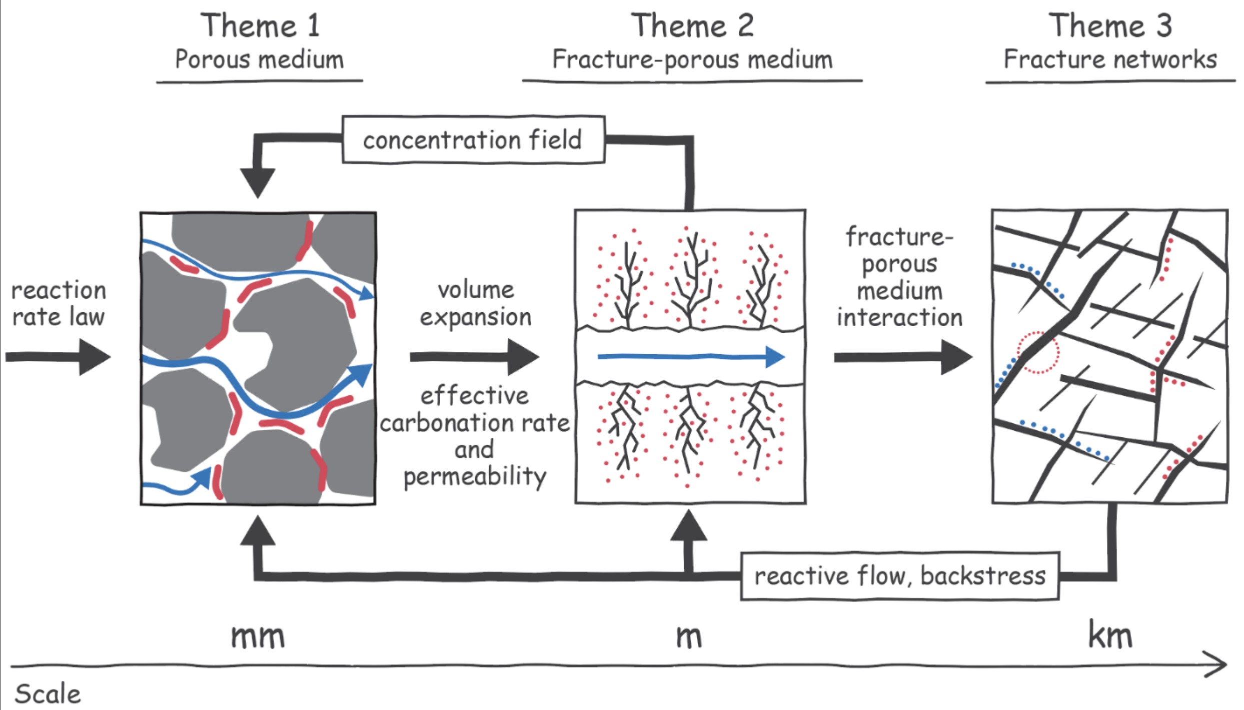
MISSION: To develop the fundamental science and engineering capability that will lead to realizing the full potential for large-scale subsurface storage of CO2 via mineralization.



gmcs.umn.edu

RESEARCH PLAN

Study the reaction, flow, and fracture processes over three distinct scales: (i) porous medium (mm) scale of the host rock, where the mineralization and carbon storage takes place; (ii) fracture-porous medium (m) scale, capturing an individual fracture from which the CO2 is delivered to the surrounding rock; (iii) fracture network (km) scale to describe how the CO2 charge is distributed by the fracture system.



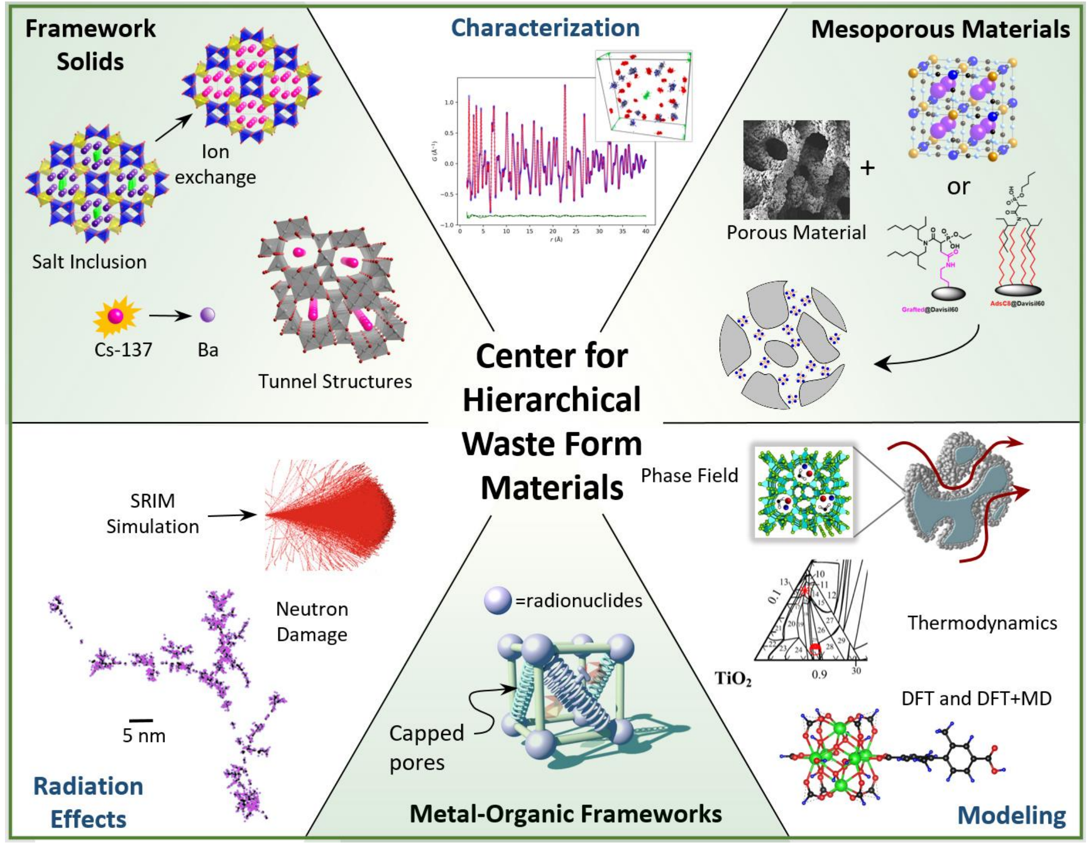
Center for Hierarchical Waste Form Materials (CHWM)

Hans-Conrad zur Loye (University of South Carolina); Class: 2016-2024

MISSION: To develop the chemical understanding and hierarchical structure motifs needed to create materials for effectively immobilizing nuclear waste species in persistent architectures.

RESEARCH PLAN

The goal of CHWM is to develop the fundamental science from which advanced waste forms for extreme and dynamic conditions can emerge. This includes 1) the development, modeling, synthesis, and demonstration of the stability of radionuclide containing hierarchical materials; 2) the direct and indirect synthetic routes for element-specific structural motifs; and 3) ion transport in multi-scale porous and hierarchical materials.



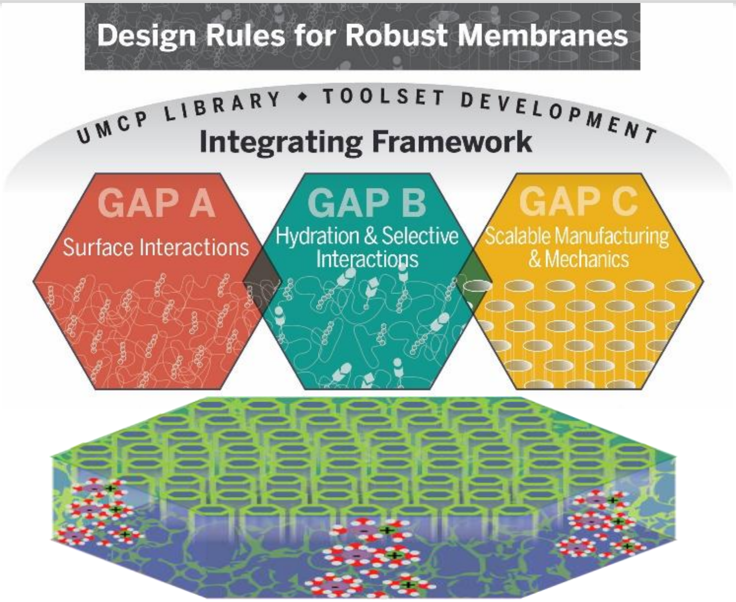
https://www.chwm.sc.edu/

The Center for Materials for Water and Energy Systems (M-WET)

Benny Freeman (The University of Texas at Austin); Class: 2018-2026

MISSION: To discover and understand the fundamental science necessary to design new membrane materials and develop tools and knowledge to predict new materials' interactions with targeted solutes to provide fit for purpose water from low quality water sources and recover valuable solutes with less energy.

https://mwet.utexas.edu/



RESEARCH PLAN

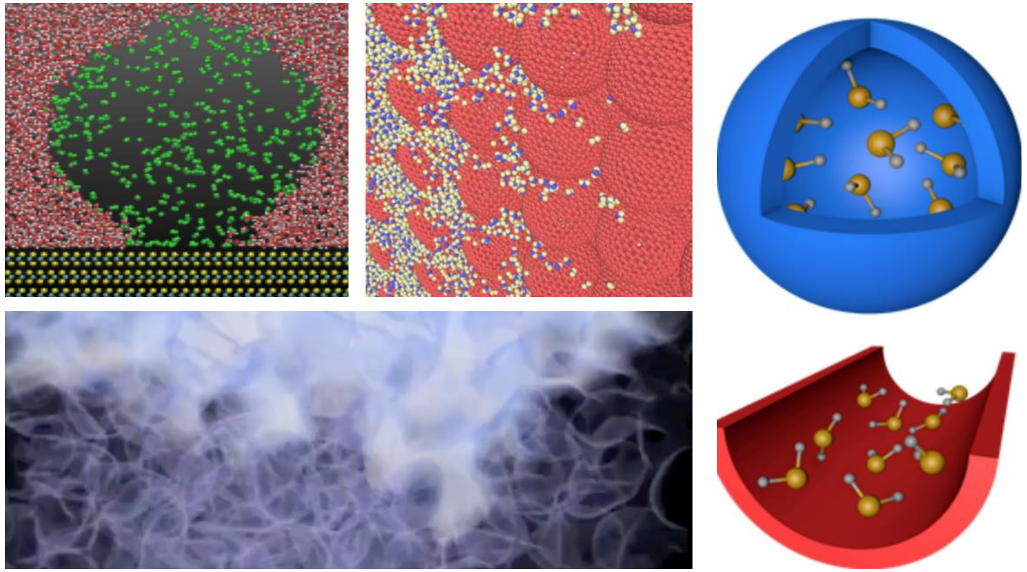
M-WET's goals are to: design new interfaces with controlled topology and functionalities; precisely control mesoscopic material architecture to build novel, highly permeable, and selective membranes with rapid, transport for resource recovery and producing fit-for-purpose water; develop novel imaging characterization tools for these systems; and model multicomponent materials, fluid mixtures, and mesoporous architectures to radically transform membrane/materials systems' energy demands, resiliency, and efficiency.

Multi-scale Fluid-Solid Interactions in Architected and Natural Materials (MUSE)

Milind Deo (University of Utah); Class: 2018-2024

MISSION: To synthesize geo-inspired materials with repeatable hierarchical heterogeneity and develop an understanding of transport and interfacial properties of fluids confined within these materials.

https://efrcmuse.utah.edu/



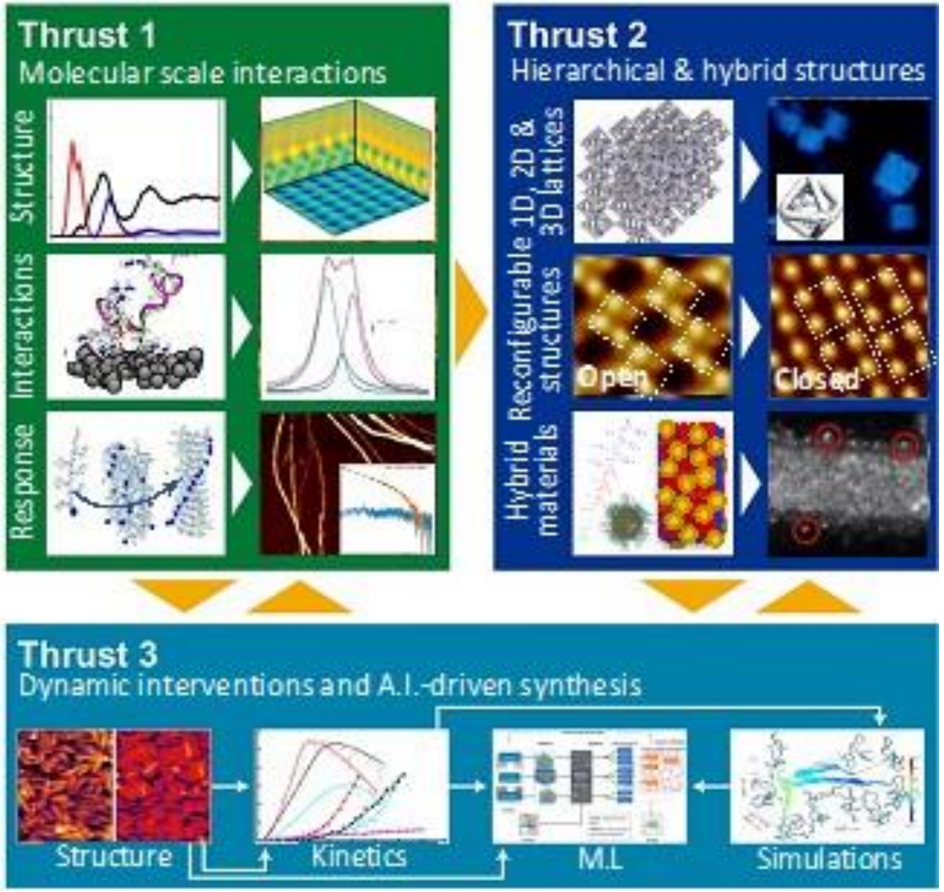
RESEARCH PLAN

Geo-inspired materials at various levels of hierarchical porosity and complexity are synthesized and used to probe thermodynamic and transport interactions of multi-phase fluids over many length scales, including at the nanometer scale. Dynamic operando measurements are performed and provide the basis for the development of experimentally-validated and atomistic-informed modeling tools and frameworks.

Center for the Science of Synthesis Across Scales(CSSAS)

François Baneyx (University of Washington); Class: 2018-2026

MISSION: To harness the complex functionality of hierarchical materials by mastering the design of high-information-content macromolecular building blocks that predictively self-assemble into responsive, reconfigurable, self-healing materials, and direct the formation and organization of inorganic components for complex energy functions.



RESEARCH PLAN

CSSAS will predict how the chemistry and sequence of inorganic, polymer and protein building blocks gives rise to ordered templates; master free energy landscapes to control the assembly of these templates into hierarchical and hybrid materials; and access new states of matter through the integration of data science, *in situ* characterization, and simulations.

https://www.cssas-efrc.com