Energy Frontier Research Centers

One Page Overviews

October 2024
https://science.osti.gov/bes/efrc

U.S. Department of ENERGY | Office of Science

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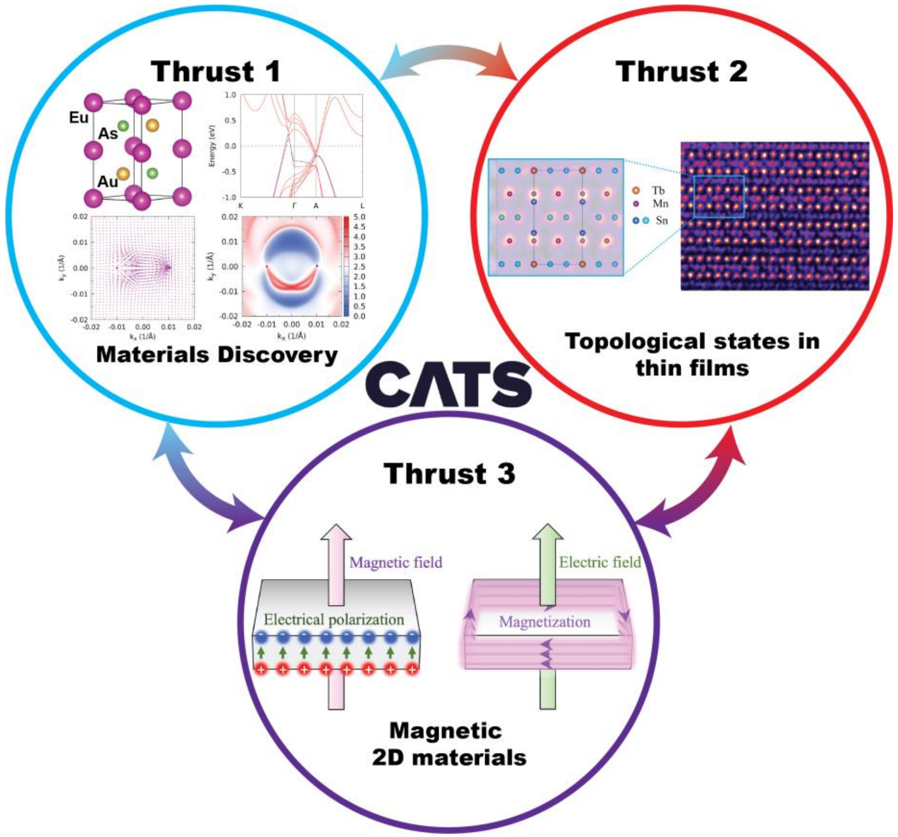
Ordered by Institution and then by Director

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 tunable layered assemblies.



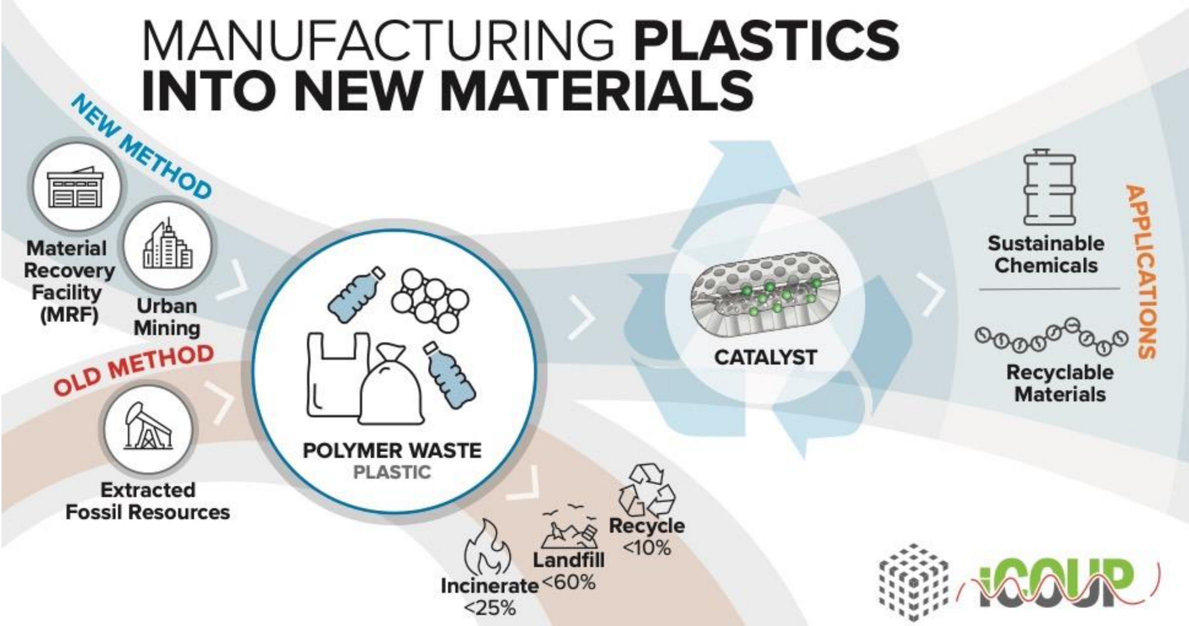
AMES NATIONAL LABORATORY Creating Materials & Energy Solutions · Argonne NATIONAL LABORATORY · BOSTON COLLEGE · HARVARD UNIVERSITY · UC SANTA BARBARA · Los Alamos NATIONAL LABORATORY · UIC UNIVERSITY OF ILLINOIS CHICAGO · UNIVERSITY OF WATERLOO · Massachusetts Institute of Technology

CATS
https://cats.ameslab.gov

Institute for Cooperative Upcycling of Plastics (iCOUP)

Aaron Sadow (Ames National Laboratory); Class: 2020-2028

MISSION: To establish the molecular and macromolecular scientific principles governing deconstruction and reconstruction of polymers to enable sustainable manufacturing from energy-rich plastics

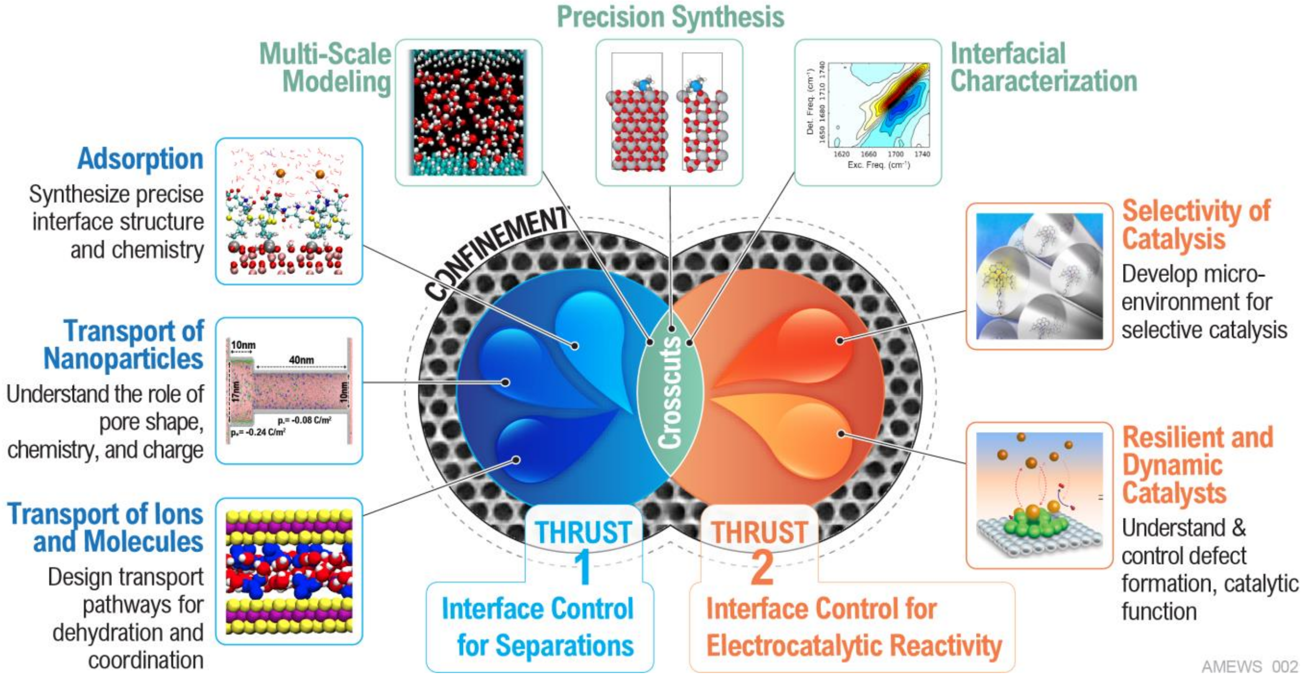


RESEARCH PLAN: iCOUP is creating inorganic catalytic materials and catalytic methods that selectively deconstruct long polymers chains into molecules of a targeted length with desired end groups. We study the fundamental molecular-, meso-, and nanoscale phenomena, such as macromolecule-catalyst interactions, underpinning these transformations. iCOUP is also investigating the chemistry to enable the use of these target molecules for the manufacture of new, value-added chemicals or recyclable polyolefins.

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

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.

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

https://www.anl.gov/amews

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

Director: Robert J. Nemanich (Arizona State University); Class: 2020 – 2026

MISSION: to understand fundamental phenomena in ultra wide bandgap (UWBG) materials – including synthesis, defect and impurity incorporation, electronic structure at interfaces, the interaction of electrons and phonons at high fields to achieve extreme electrical properties, and phonon phenomena that affect thermal transport. The Future Grid Co-Design Ecosystem enables communication across all levels of the science and technology.

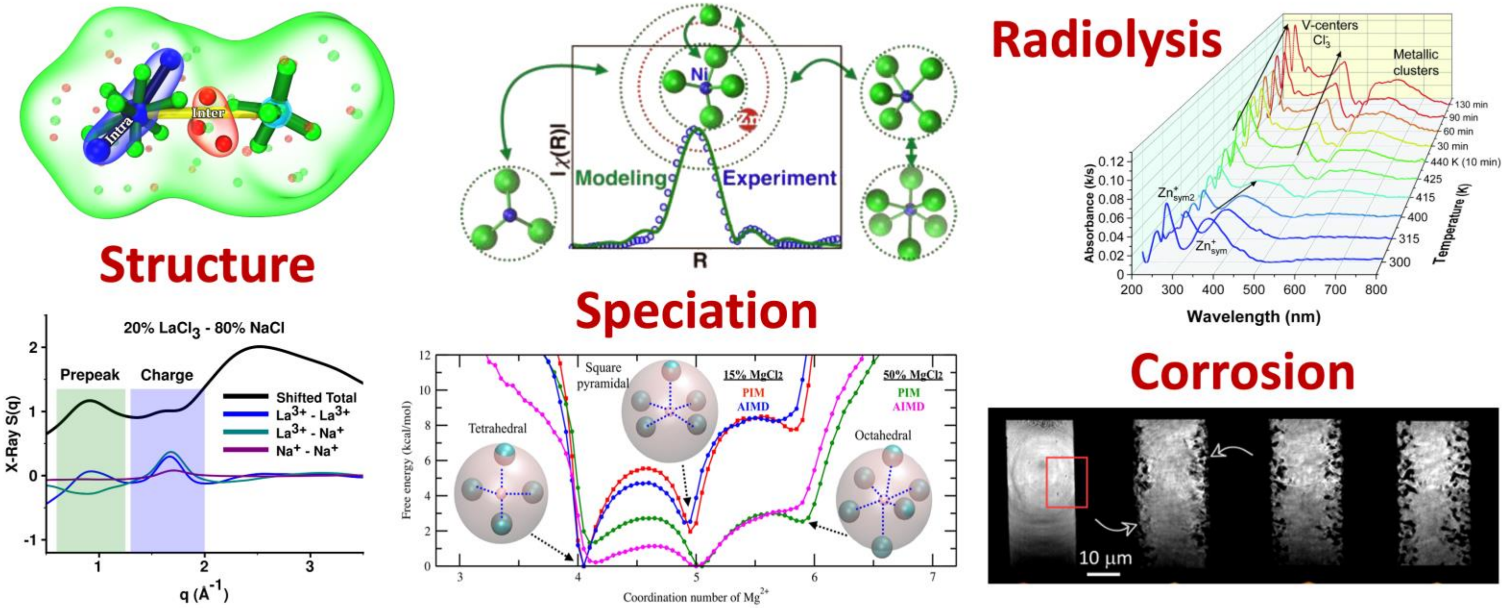
RESEARCH PLAN: Specific outcomes include: 1) scalable synthesis of cubic and hexagonal UWBG semiconductors and effective doping using their unique properties, 2) synthesized UWBG heterostructures with designed interface electronic properties, 3) demonstration of high electric-field breakdown and high current transport in UWBG semiconductors, 4) optimized electron-phonon interactions for efficient thermal transport in UWBG materials and importantly, their interfaces, and 5) predictive assessment of UWBG materials in power electronics and the electric grid network.

https://ultracenter.asu.edu/

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.



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.

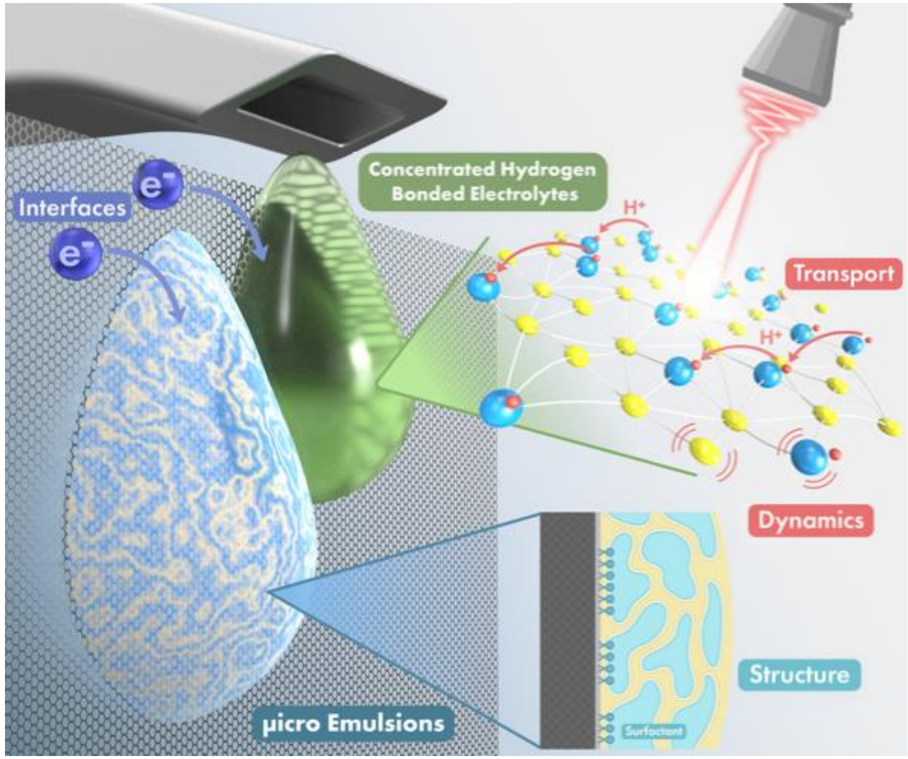
https://www.bnl.gov/moltensalts

MSEE molten salts in extreme environments · Brookhaven National Laboratory · INL Idaho National Laboratory · Oak Ridge National Laboratory · The University of Tennessee Knoxville · Stony Brook University · The University of Iowa · University of Notre Dame · University of Michigan · Wisconsin University of Wisconsin-Madison

Breakthrough Electrolytes for Energy Storage and Systems (BEES2)

Burcu Gurkan (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

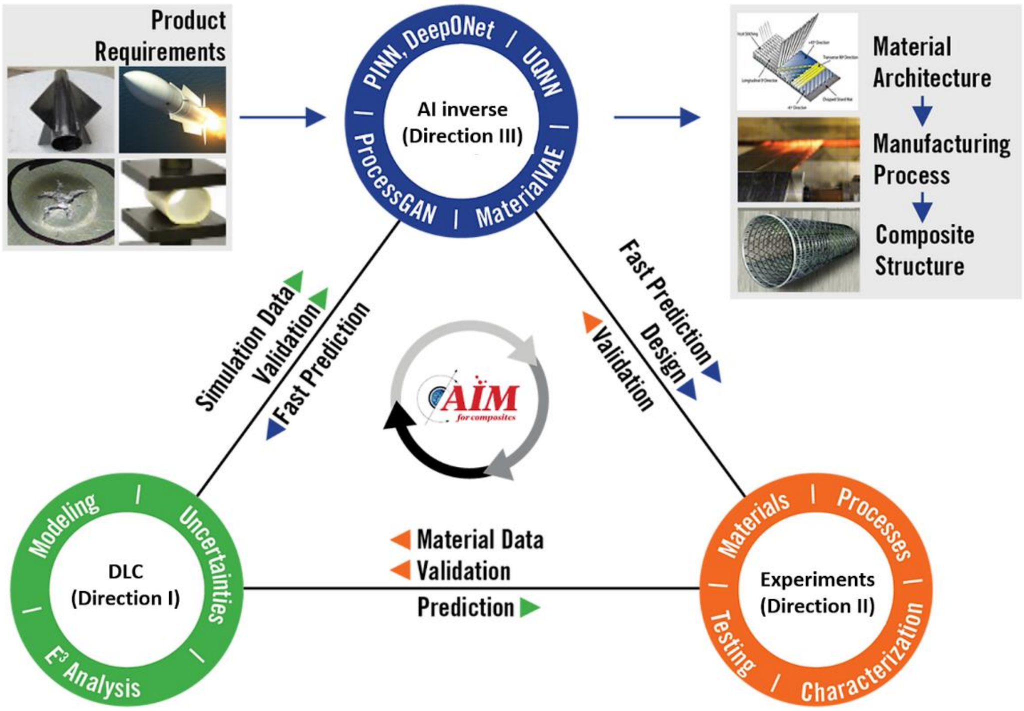
BEES2 | NYU | HUNTER The City University of New York | Case Western Reserve University EST. 1826 | University of Notre Dame | University of Illinois Urbana-Champaign | The University of Tennessee Knoxville | A&M | The Ohio State University

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 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://aimforcomposites.com/

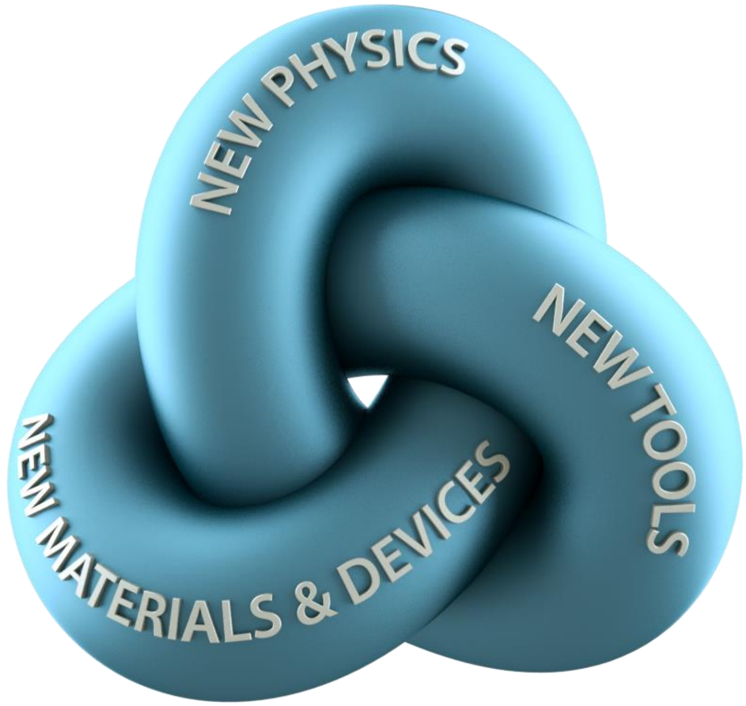
Clemson University · University of Delaware · UF University of Florida · Ohio State · Brown · SC State University · Pacific Northwest National Laboratory · Savannah River National Laboratory

Programmable Quantum Materials (Pro-QM)

Dimitri 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

COLUMBIA UNIVERSITY IN THE CITY OF NEW YORK

Brookhaven National Laboratory

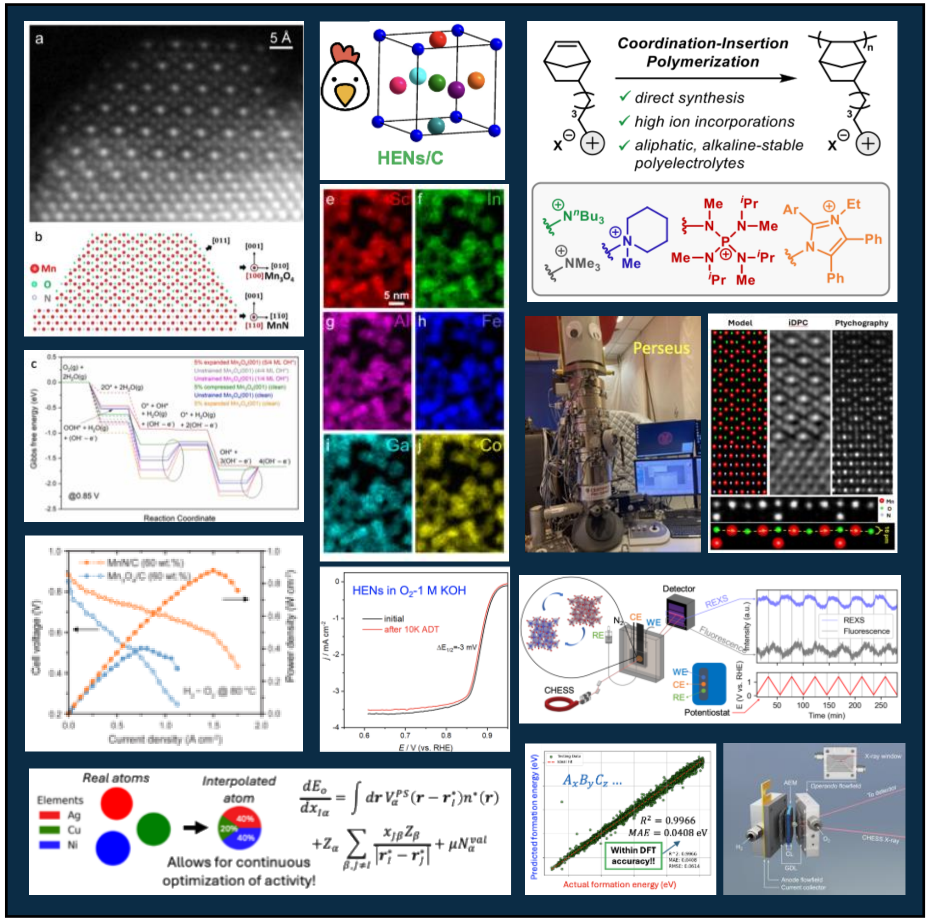
Pro-QM Programmable Quantum Materials DOE Energy Frontiers Research Center

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.

RESEARCH PLAN: Alkaline media enables electrochemical energy conversion technologies that can employ only abundant elements. ***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. Our work is enabled by a synergistic research approach that integrates theory, computational methods, machine learning and artificial intelligence, synthesis of electrocatalysts and novel membrane materials and the development and use of novel experimental tools to provide *in situ/operando*, spatiotemporal characterization of systems under operation.



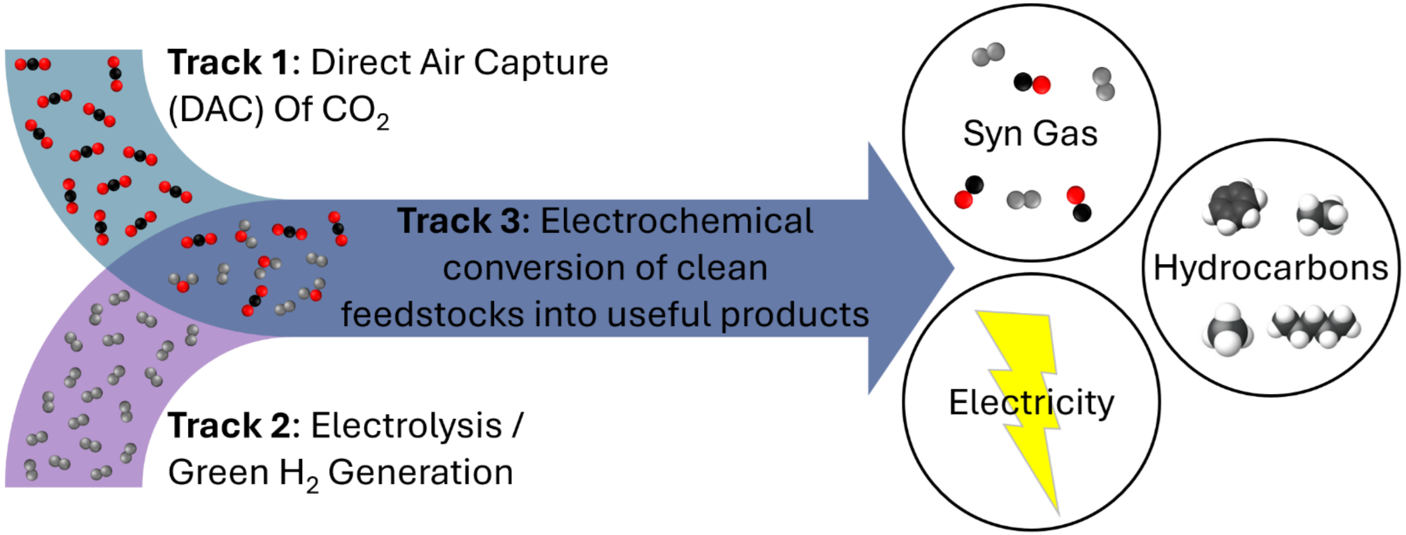
cabes.cornell.edu

CABES Center for Alkaline-based Energy Solutions | Cornell University | Carnegie Mellon University | Los Alamos National Laboratory | NREL | PennState | Penn | Princeton University | UTEP | The University of Wisconsin Madison

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.



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.

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

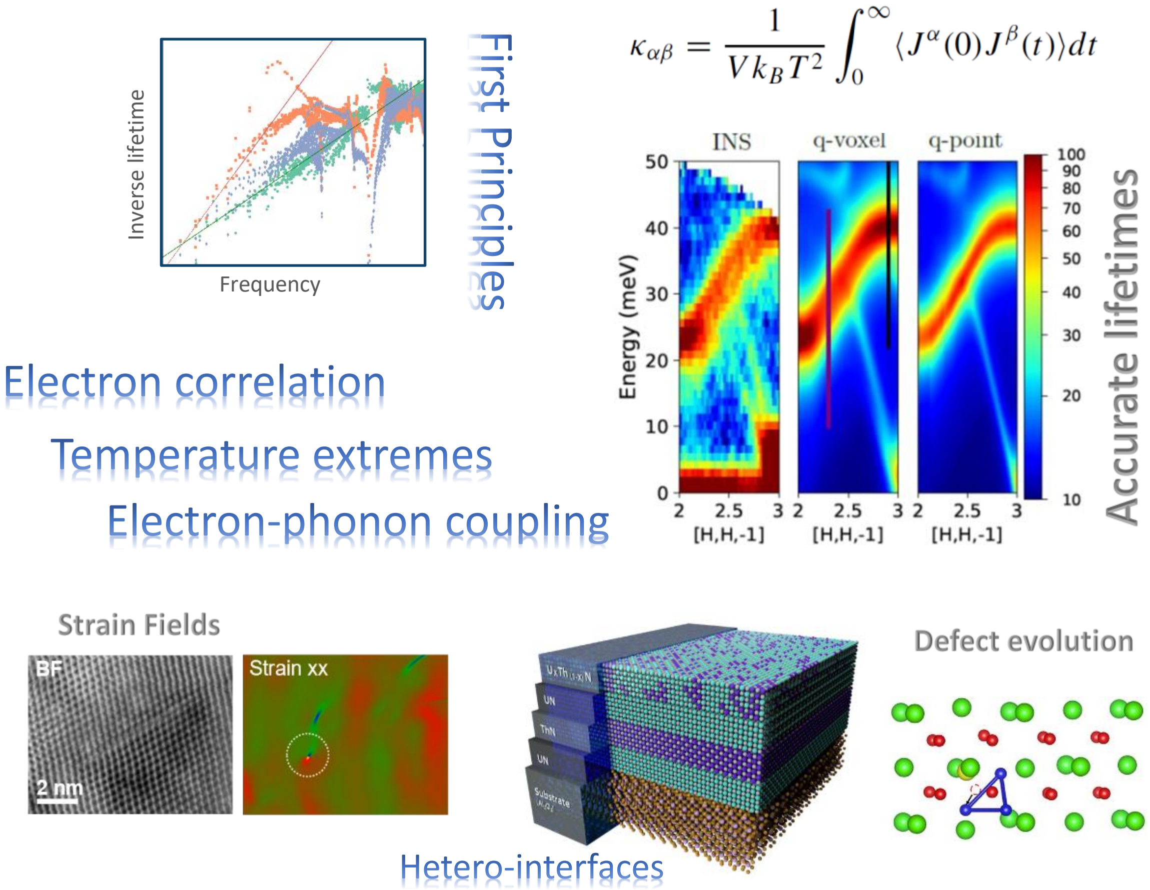
UNCAGE ME | Georgia Institute of Technology | Oak Ridge National Laboratory | The University of Alabama | UF University of Florida | Sandia National Laboratories | USC University of Southern California | University of Michigan | Lehigh University

Center for Thermal Energy Transport under Irradiation (TETI)

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

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

RESEARCH PLAN: The transport of heat (thermal energy) 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 engineers the necessary tools to design advanced nuclear fuel by tailoring defects and microstructure.



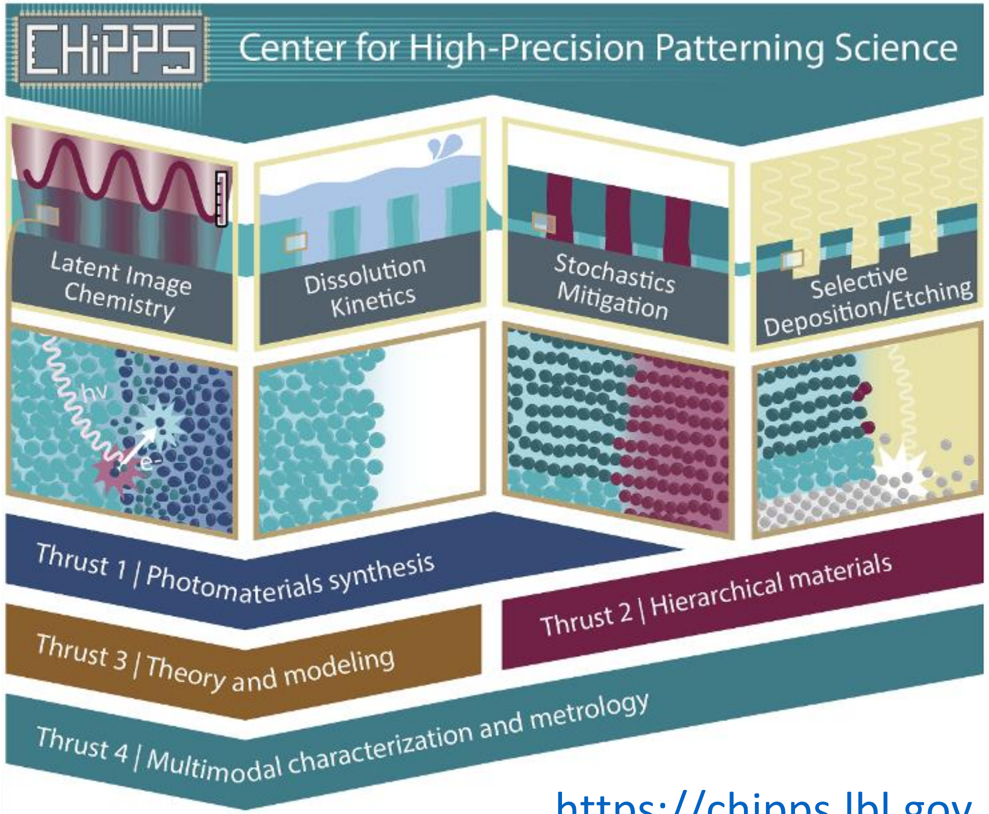
http://teti.inl.gov

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

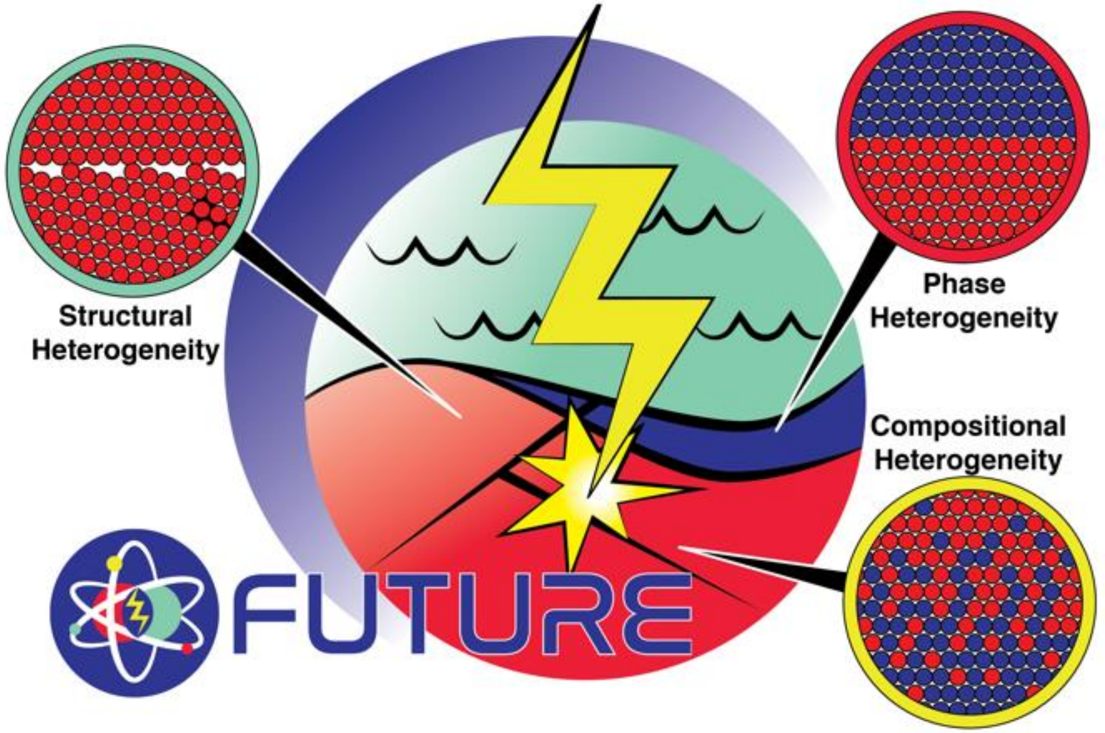
Stanford University · Cornell University · Argonne National Laboratory · SJSU San José State University · UC Santa Barbara · Berkeley Lab

Fundamental Understanding of Transport Under Reactor Extremes (FUTURE)

Blas 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.

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 and govern their irradiation and corrosive evolution.



https://m.lanl.gov/future

Center for Enhanced Nanofluidic Transport – Phase 2 ($CENT^2$)

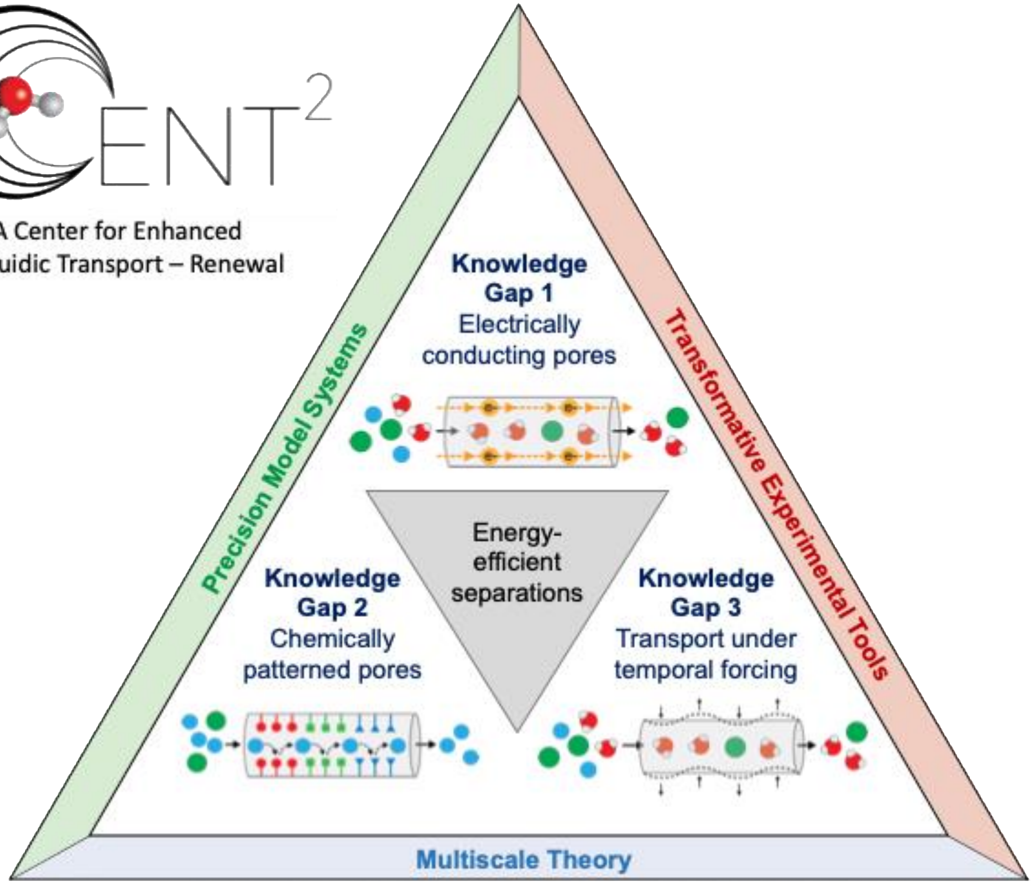
Michael S. Strano (Massachusetts Institute of Technology); Class: 2018-2026

MISSION: To address critical knowledge gaps in our understanding of fluidic flow and molecular transport in single-digit nanopores. $CENT^2$ will establish the scientific foundation for transformative molecular separation technologies impacting the water-energy nexus.

RESEARCH PLAN: $CENT^2$ will apply precision model systems, transformative experimental tools, and predictive multiscale theories to understand fluid flow and molecular transport in single-digit nanopores. These insights will allow us 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.

https://cent.mit.edu/

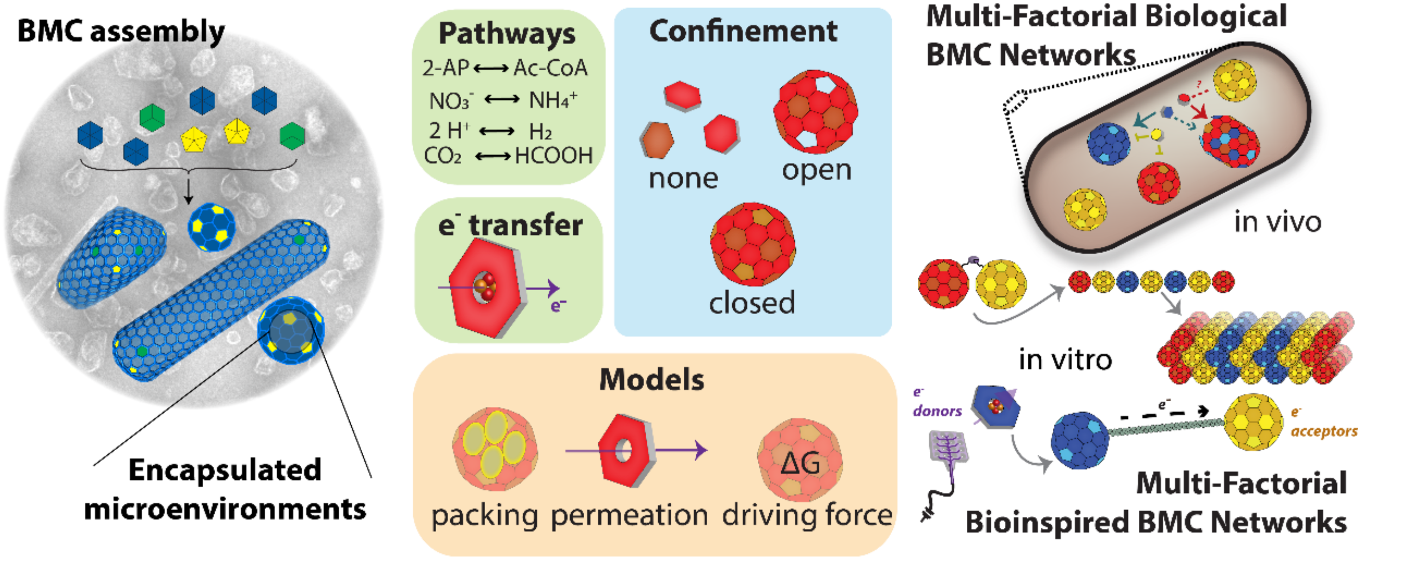
EFRC: A Center for Enhanced Nanofluidic Transport – Renewal



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.



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) and to 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.

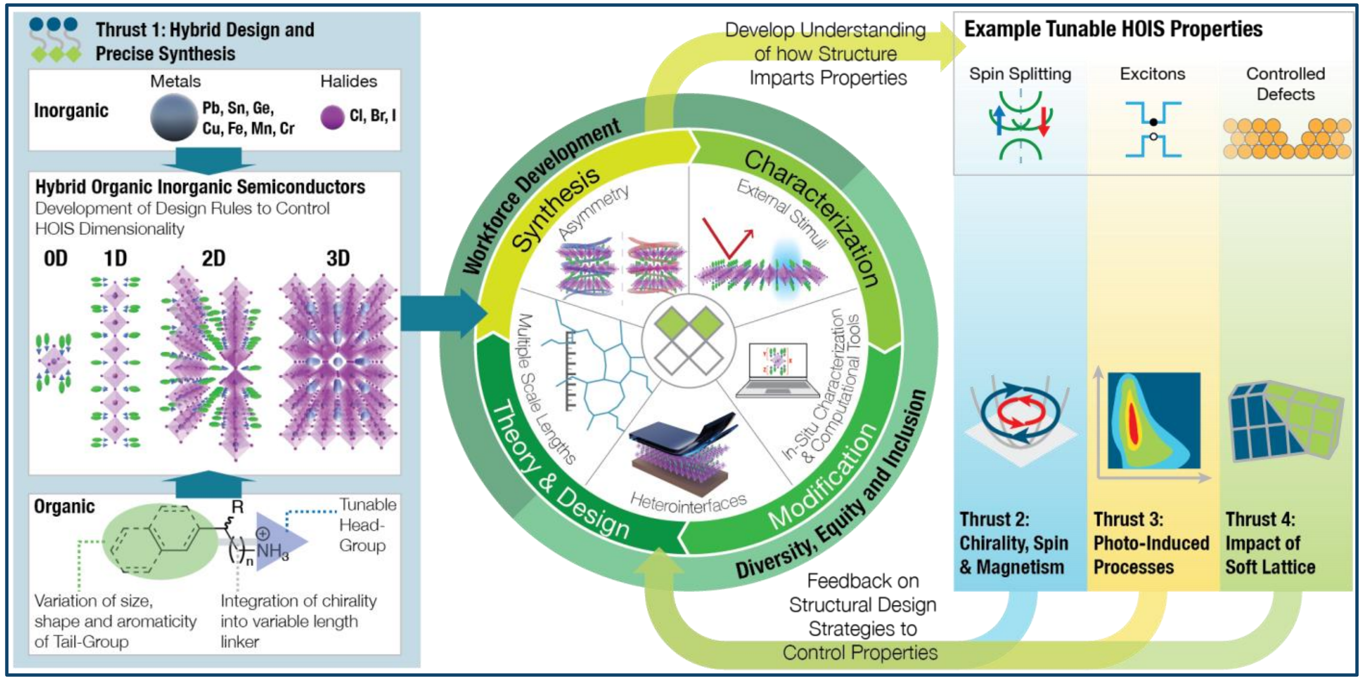
https://www.ccbc-efrc.org/

Center for Catalysis in Biomimetic Confinement · Michigan State University · Argonne National Laboratory · Berkeley Lab

Center for Hybrid Organic Inorganic Semiconductors for Energy (CHOISE)
Matthew C. Beard (NREL); Class: 2018-2026

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

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.

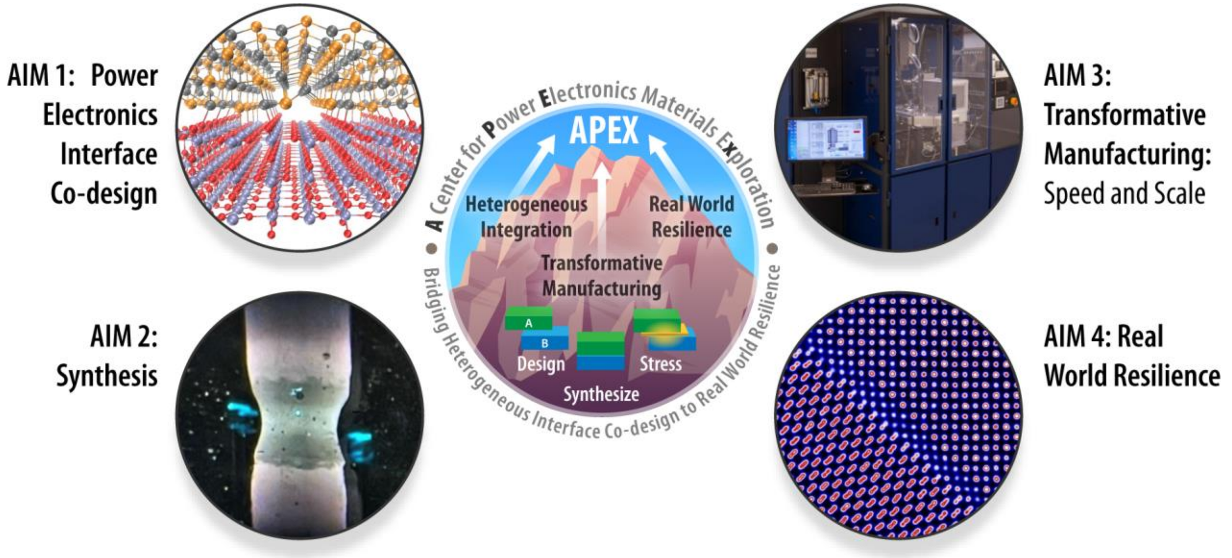


www.choise-efrc.org

A Center for Power Electronics Materials and Manufacturing Exploration (APEX)

Nancy M. Haegel (NREL); Class: 2024-2028

MISSION: To expand interdependent materials and manufacturing choices for substrates, ultrawide-bandgap semiconductors, contacts, thermal sinks, and critical interfacial layers and advance fundamental understanding of structurally, chemically, thermally, and electrically dissimilar interfaces.

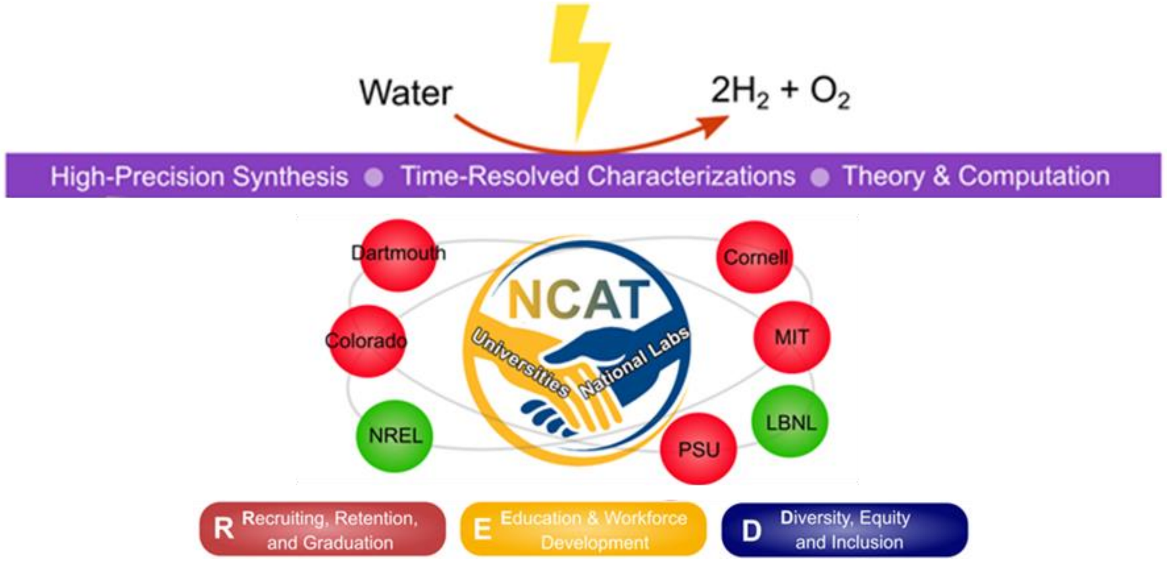


RESEARCH PLAN: Next-generation power conversion technologies have the potential to significantly improve energy efficiency and reduce global energy consumption. APEX focuses on four areas of research: (1) co-design of interfaces for broader integration of heterogeneous materials, (2) synthesis of novel materials combinations, (3) transformative manufacturing through hydride vapor phase epitaxy for speed and scale, and (4) understanding of interfacial phases, reactions, and degradation mechanisms to further knowledge for real-world performance and resilience.

APEX A Center for Power Electronics Materials and Manufacturing Exploration | NREL National Renewable Energy Laboratory | Morgan State University | Johns Hopkins University | Colorado School of Mines | University of Virginia | Argonne National Laboratory | Kyma technologies

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.

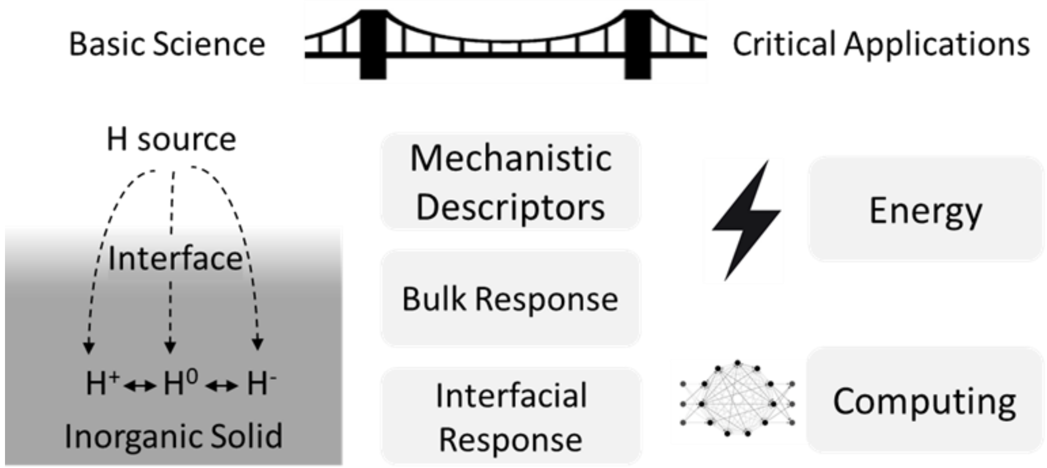
www.cedars-ncat.org

North Carolina A&T State University · University of Colorado Boulder · Dartmouth · MIT · Cornell · Berkeley Lab · NREL

Hydrogen in Energy and Information Sciences (HEISs)

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

MISSION: HEISs aims 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).



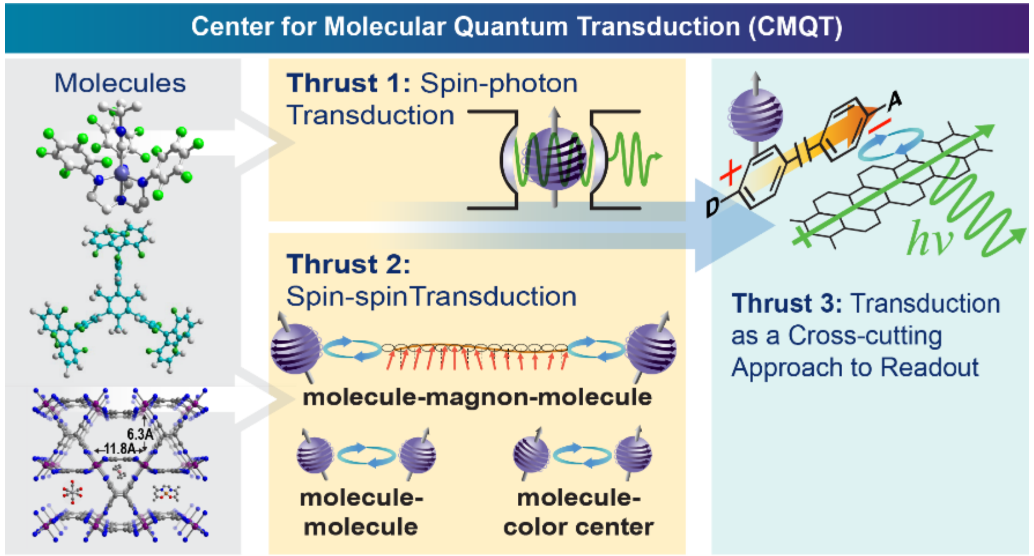
RESEARCH PLAN: Leveraging the interdisciplinary expertise of the team, which spans from chemistry to materials science, and applied physics to nuclear engineering, HEISs undertakes comprehensive studies to assess hydrogen (H^+, H^0, and H^-) transport through **bulk** materials, across and along solid-solid **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 – to manipulate, enhance, and exploit hydrogen dynamics.

https://heiss.northwestern.edu/

Center for Molecular Quantum Transduction (CMQT)

Michael R. Wasielewski, Director (Northwestern University); Class: 2020-2028

MISSION: Quantum transduction is the coherent exchange of information between quantum systems, which is an essential element of quantum information science. The mission of **CMQT** is to develop the fundamental scientific understanding needed to conduct quantum-to-quantum transduction through a bottoms-up synthetic approach that imparts atomistic precision to quantum systems.



RESEARCH PLAN

- Investigate spin-photon transduction in hybrid materials at both the ensemble and single molecule levels.
- Explore spin-spin transduction in hybrid materials as a modular and generalized approach to exchanging quantum information between dissimilar quantum systems.
- Develop new strategies for employing transduction to enhance the readout of quantum information encoded in molecular spin qubits.

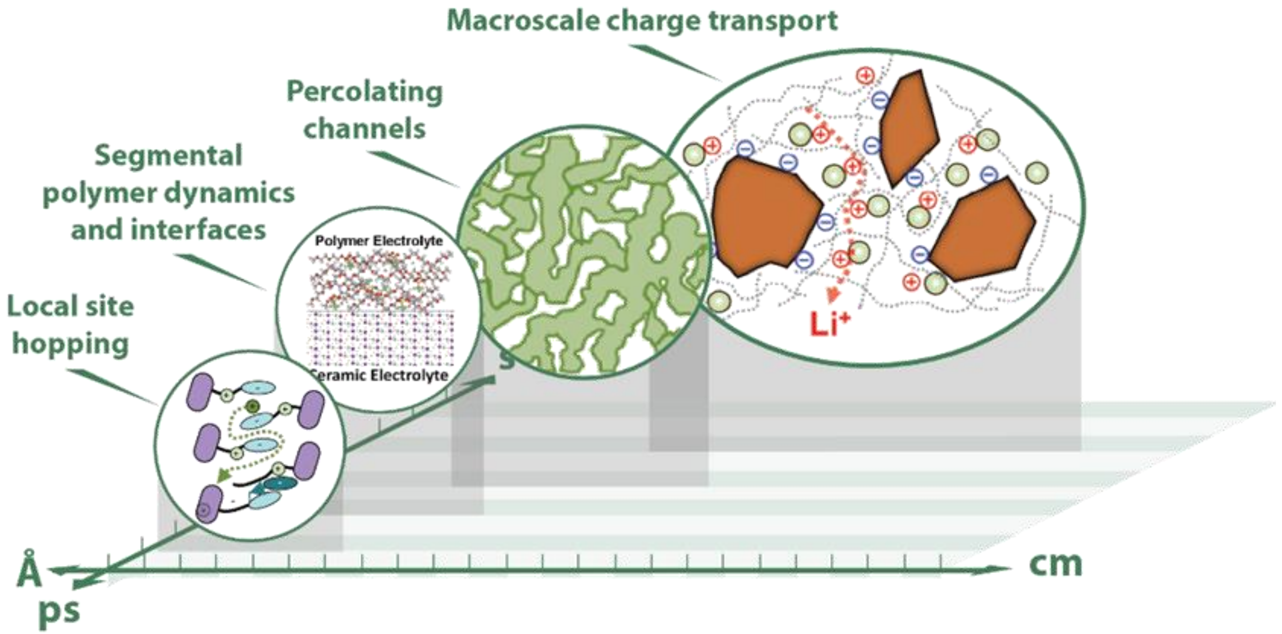
https://cmqt.org

CMQT CENTER FOR MOLECULAR QUANTUM TRANSDUCTION

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

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.

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.

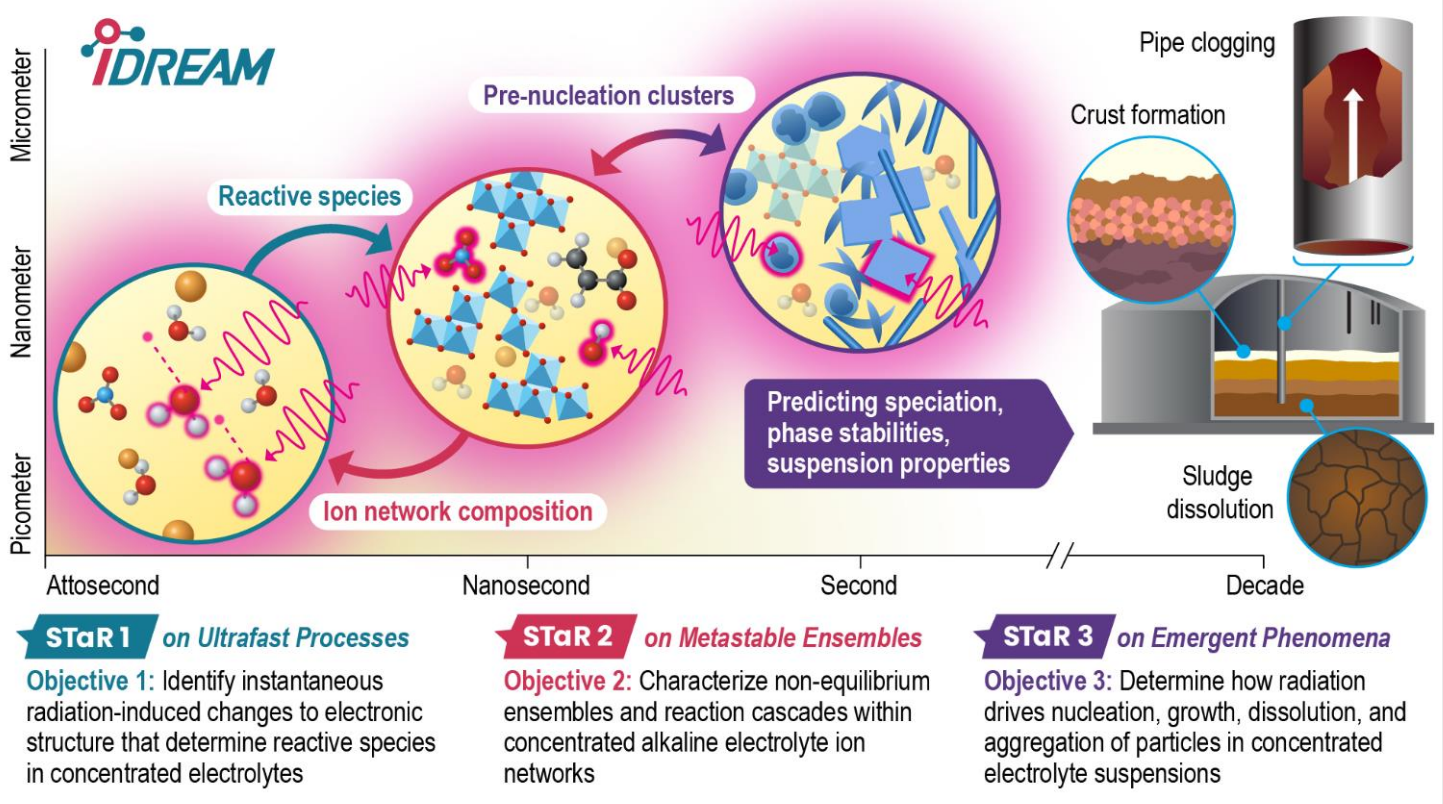
https://fact-efrc.ornl.gov/

Ion Dynamics in Radioactive Environments and Materials (IDREAM)

Carolyn Pearce (Pacific Northwest National Laboratory); Class: 2016-2028

MISSION: To master the cascade of radiation chemistry that drives far from equilibrium speciation and reactivity in chemically complex environments, linking attosecond timescales to decadal processes.

RESEARCH PLAN: Provide the technical basis to improve retrieval and processing of millions of gallons of radioactive tank waste at DOE legacy sites and to inform treatment of waste from new nuclear reactors. Combine experimental and computational expertise to revolutionize the manipulation of chemical processes in extreme far from equilibrium environments that are characterized by high ionic strength and radiation-induced metastability across different spatiotemporal regimes (STaRs).



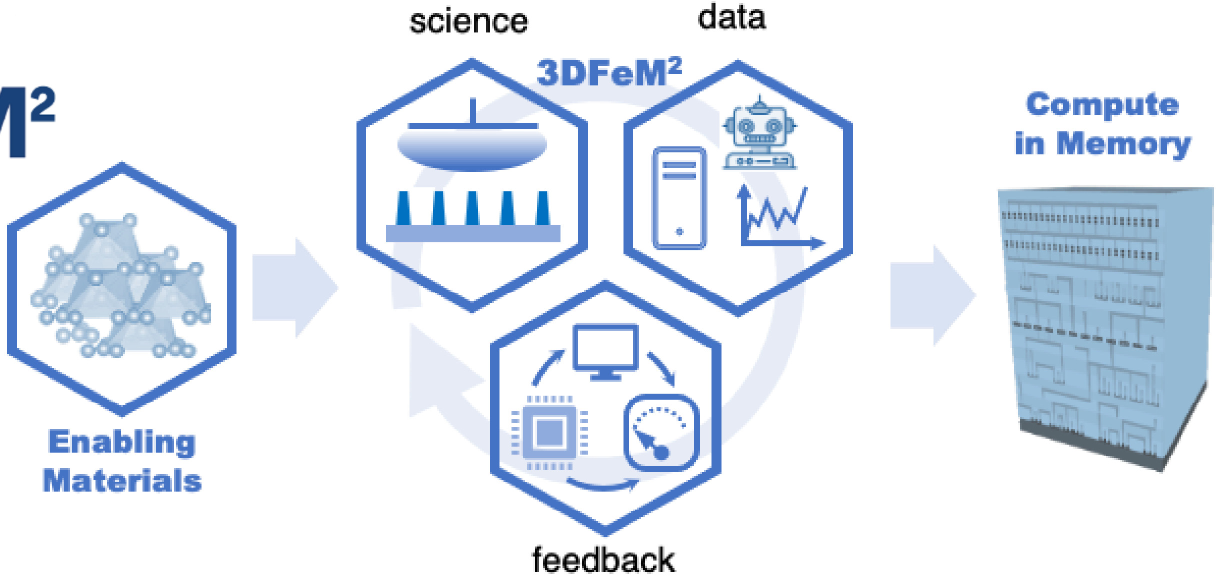
www.pnnl.gov/idream

IDREAM Pacific Northwest National Laboratory Argonne National Laboratory Oak Ridge National Laboratory Georgia Tech HUNTER The City University of New York University of Notre Dame The University of Utah University of Washington

Center for 3 Dimensional Ferroelectric Microelectronics Manufacturing ($3DFeM^2$)

Susan Trolier-McKinstry (The Pennsylvania State University); Class: 2020-2028

MISSION: To integrate reliable, scaled ferroelectric films for 3D memory using next generation manufacturing practices. Autonomous experiments and machine learning (ML) will expedite optimization; digital twins accelerate innovation through virtual experiments.



RESEARCH PLAN: $3DFeM^2$ will ***i.*** understand crystal chemistry design rules and boundary conditions that regulate ferroelectricity, ***ii.*** control ferroelectricity-enabling and lifetime-limiting defects in next-generation ferroelectrics, ***iii.*** identify descriptors for defect chemistry, structure, and property evolution during processing, ***iv.*** utilize ML and *in situ* microscopy to identify phases, switching mechanisms, and scaling trends, ***v.*** enable autonomous workflows for 3D film growth and etching, ***vi.*** generate novel device concepts, and ***vii.*** establish predictive digital twins based on device configuration, manufacturing process history and system-level operation.

https://3dfem.psu.edu/

PennState, Georgia Tech, University of Virginia, The University of Tennessee Knoxville, University of Notre Dame, Penn University of Pennsylvania, University of Maryland, Carnegie Mellon University, Brookhaven National Laboratory, Oak Ridge National Laboratory, Sandia National Laboratories

Bioinspired Light-Escalated Chemistry (BioLEC)

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

MISSION: To combine light harvesting and solar photochemistry to enable more powerful editing, building, and transforming of abundant materials to produce energy-rich feedstock chemicals.

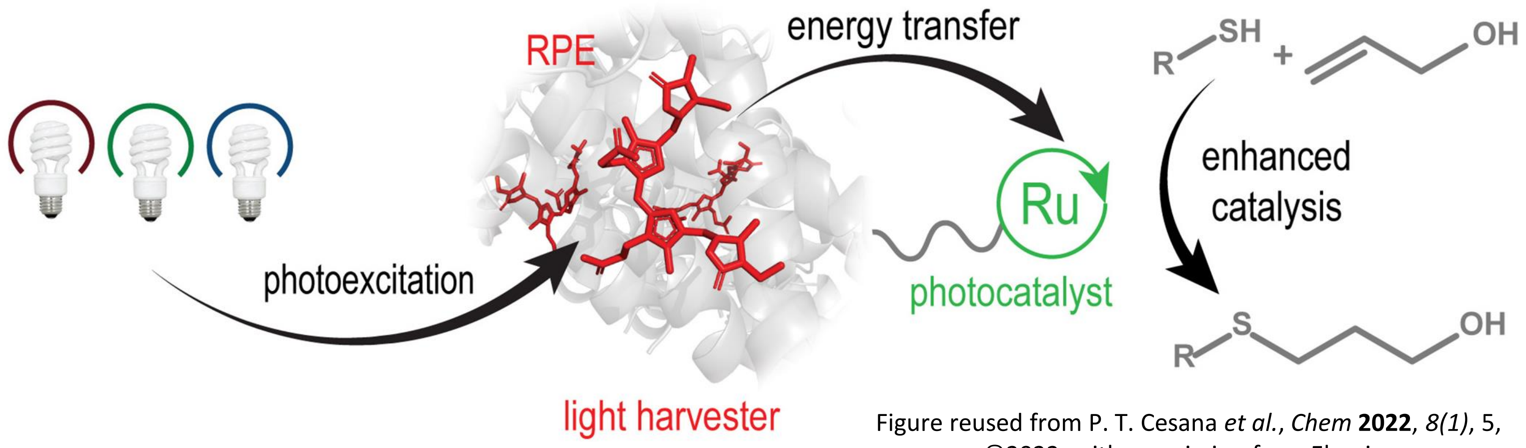


Figure reused from P. T. Cesana *et al.*, *Chem* **2022**, *8(1)*, 5, ©2022, with permission from Elsevier

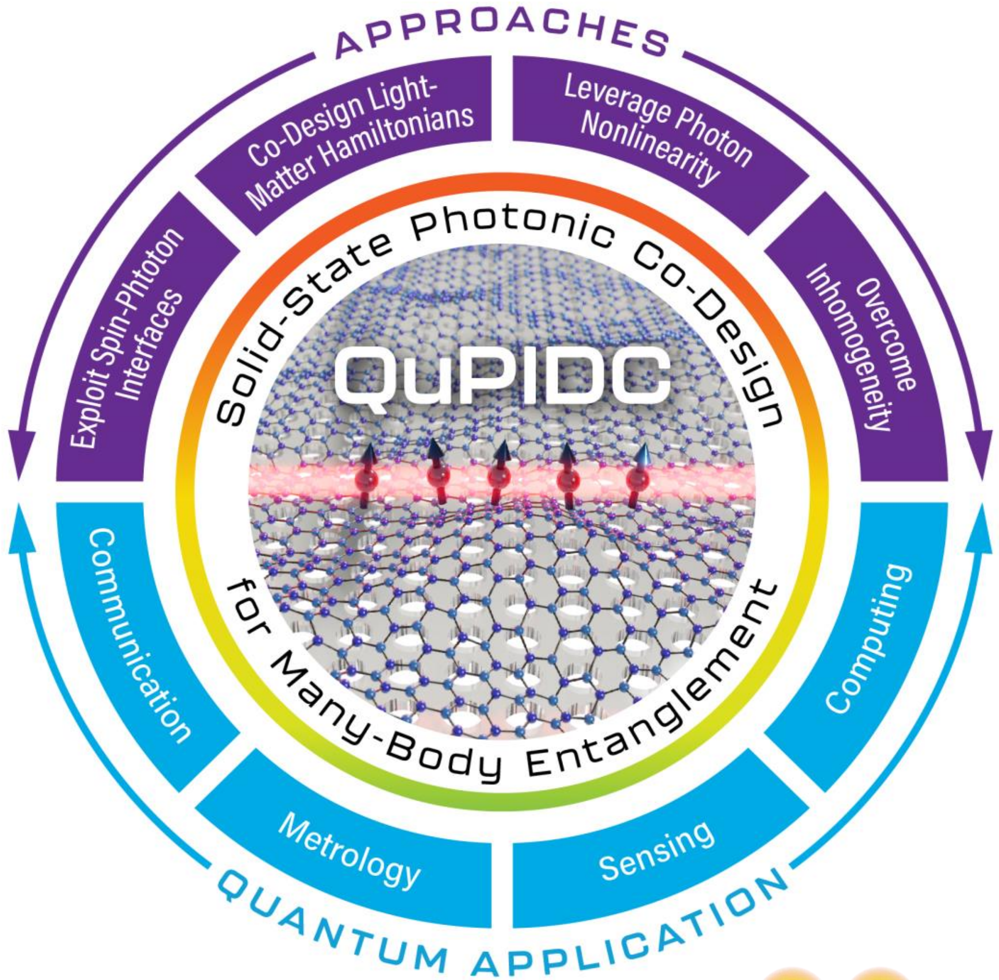
RESEARCH PLAN: We aim to reduce the energy costs of chemical manufacturing by finding ways to replace fossil fuels as both energy source and starting materials. We tackle this by developing photochemistry that enables new routes for synthesizing chemical feedstocks using only light for energy; looking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

Quantum Photonic Integrated Design Center (QuPIDC)

Libai Huang (Purdue University); Class: 2024-2028

MISSION: To discover, design, and realize robust many-body entangled photon and matter states through multi-scale co-designing strategies in heterogeneous solid-state photonic systems.

RESEARCH PLAN: By co-designing systems' Hamiltonians including both the emitters and their photonic environments to control coherence and entanglement processes within heterogeneous materials, QuPIDC will realize a variety of quantum state of photons that are robust against inhomogeneity, decoherence and loss.

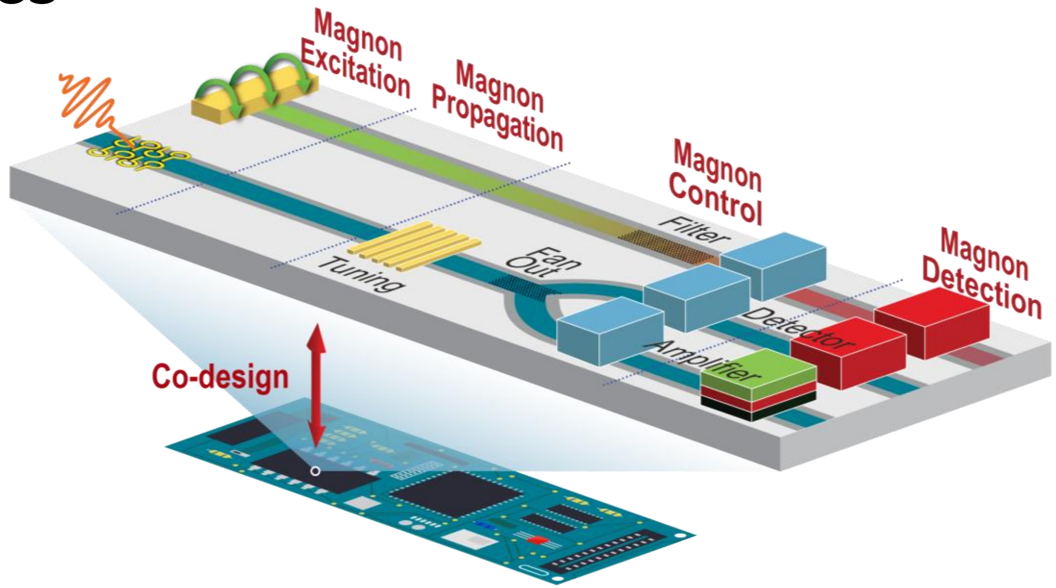


PURDUE UNIVERSITY · Los Alamos National Laboratory EST. 1943 · Stanford · Northwestern University · The University of Chicago · OU · UMBC · Virginia Tech · NC State University · QuPIDC

https://www.science.purdue.edu/qupidc/

Center for Energy Efficient Magnonics

Yuri Suzuki (SLAC); Class: 2024-2028



MISSION: To advance the basic scientific understanding of magnon excitation, propagation, transduction, and control that is motivated by an end use of magnon-based interconnects and their integration into microelectronics.

RESEARCH PLAN: Magnons provide the promise for microelectronics with low-loss information and energy transfer at the nanoscale using propagating excitations with wavelengths that are orders of magnitude smaller than microwave or photonic interconnects. We will (i) manufacture resilient ferrimagnetic and antiferromagnetic materials with record low damping, (ii) demonstrate robust tunability of these materials to functionalize magnon interconnects, (iii) enhance magnon transmission among and within these materials and at interfaces, (iv) generate and detect coherent and incoherent magnons efficiently from GHz to THz frequencies, (v) develop a framework for nonlinear magnon behavior.

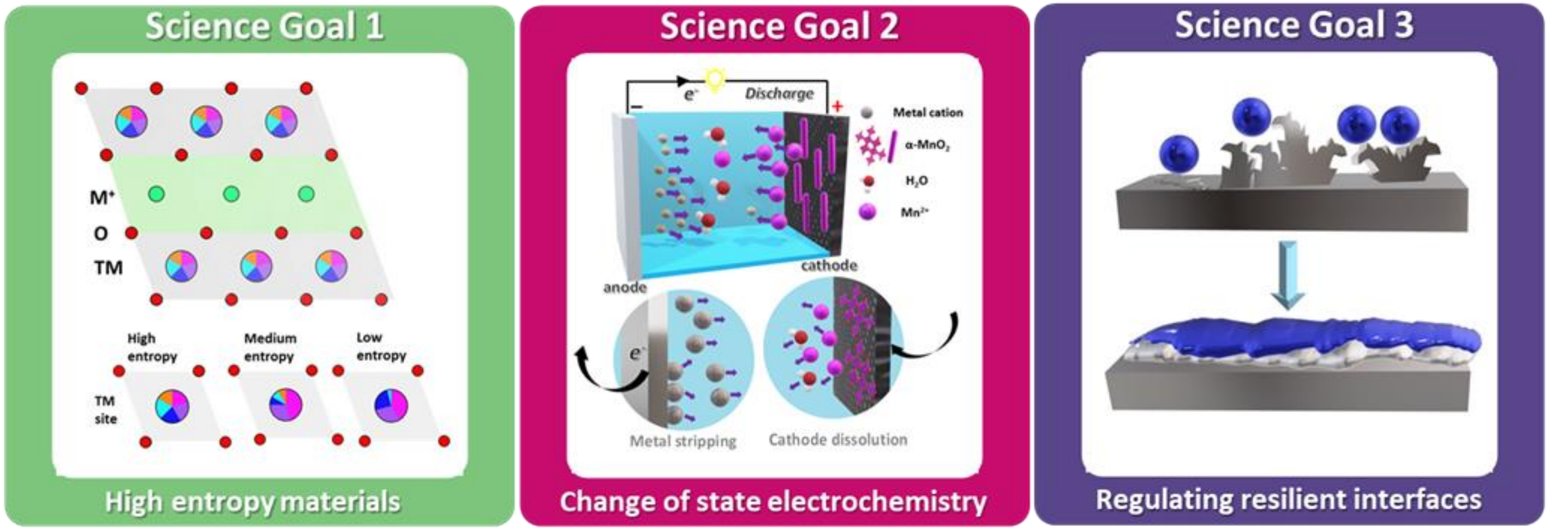
CEEMag
https://ceemag.slac.stanford.edu

SLAC | Stanford | Cornell | Morgan State University | Northwestern | The Ohio State University | UCI University of California, Irvine | IOWA | TEXAS The University of Texas at Austin

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.



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 | Lehigh University | Texas, The University of Texas at Austin | Xavier University of Louisiana

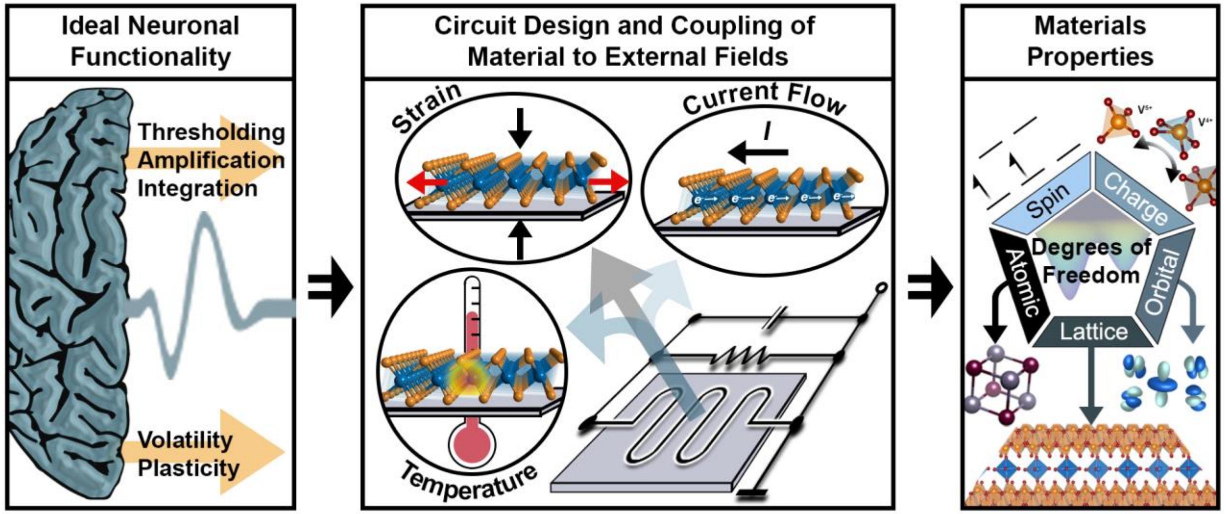
m2m#s molecular to mesoscale

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

Reconfigurable Electronic Materials Inspired by Nonlinear Neuron Dynamics (REMIND)

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

MISSION: Establish foundational scientific knowledge underpinning the *function of reconfigurable materials, devices, and computing architectures* that approach *fundamental limits of energy efficiency and speed* to enable emulation of specific neuronal and synaptic functions of the human brain.



RESEARCH PLAN: REMIND will flip the current computing paradigm by blending inverse & forward design, material synthesis & manipulation, and development of advanced in-situ & operando characterization tools to connect dynamical material properties and underlying transformations in reconfigurable, nonlinear electronic materials. We will discover molecular/material building blocks and exploit fundamental mechanisms in new materials and at tailored interfaces that are required to emulate specific neuronal and synaptic functions and enable a new paradigm of brain-inspired computing.

https://remind.engr.tamu.edu/

reMIND

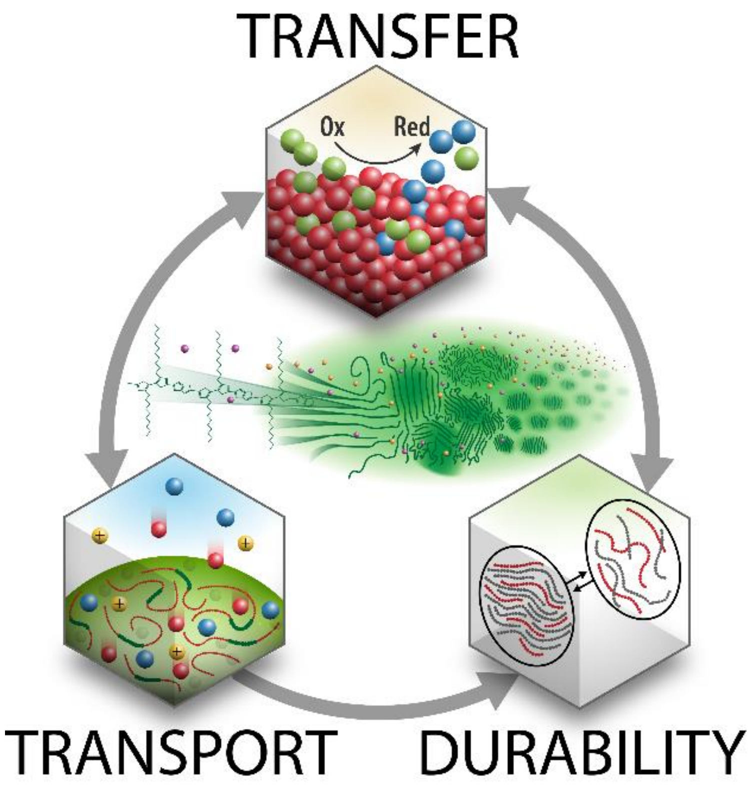
Texas A&M Engineering Experiment Station | NREL Transforming ENERGY | Sandia National Laboratories | BERKELEY LAB

Center for Soft PhotoElectroChemical Systems (SPECS)

Neal Armstrong (University of Arizona); Class: 2022-2026

MISSION: SPECS understands the factors controlling charge and matter transport processes in inexpensive, scalable, and durable π-conjugated polymer (plastic) materials. We 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.

RESEARCH PLAN: SPECS is organized around 3 interconnected thrusts that focus on energy conversion and storage systems. ***Thrust 1: Hybrid Electrical-Ionic Charge Transport*** understands and controls the complex polymer/electrolyte structures that control ion and charge transport. ***Thrust 2: Charge Transfer and Energy Cascades*** understands and optimizes 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 robust design guidelines.



https://specs.arizona.edu

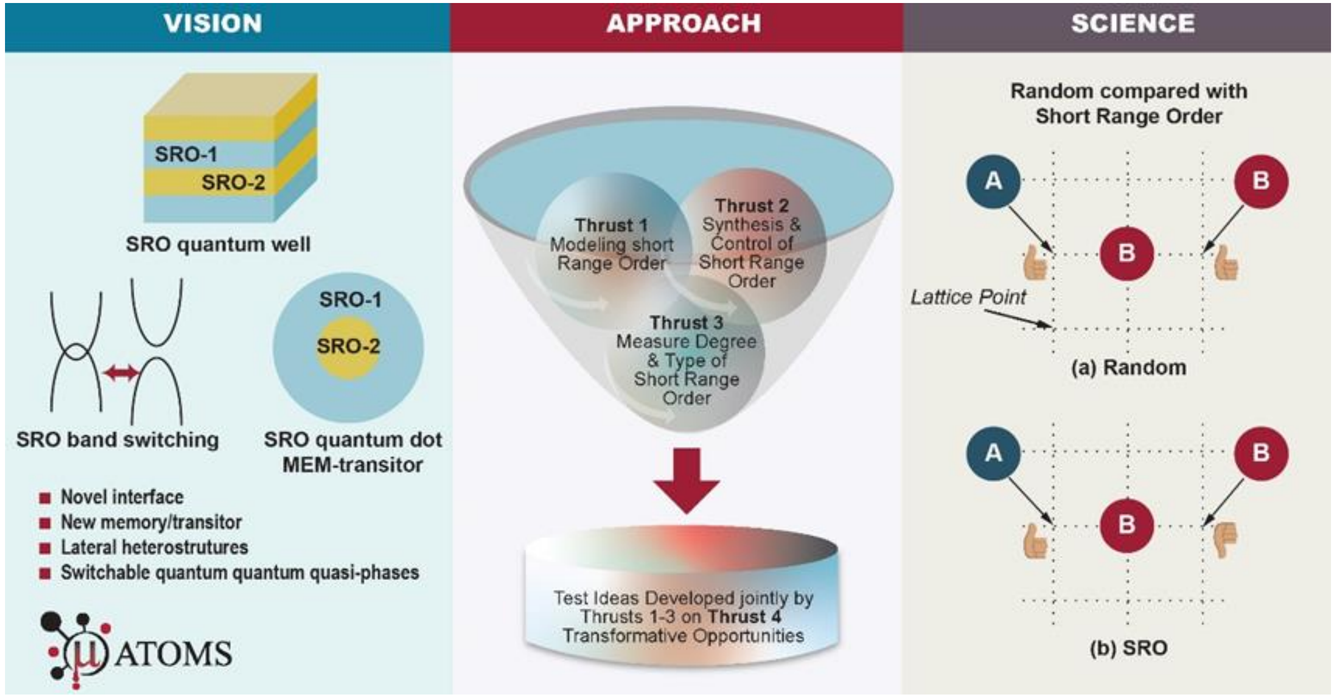
SPECS · The University of Arizona · NREL Transforming ENERGY · University of Colorado Boulder · Emory University · UK · Georgia Tech

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.

RESEARCH PLAN: µ-ATOMS models both material and structure to guide fabrication, develops and demonstrates new synthesis tools and techniques, uses a suite of new characterization tools to develop the measurement ability, and controls atomic order in semiconductor alloys for transformative opportunities enabled by the new optical, electrical, quantum, and structure transition properties.



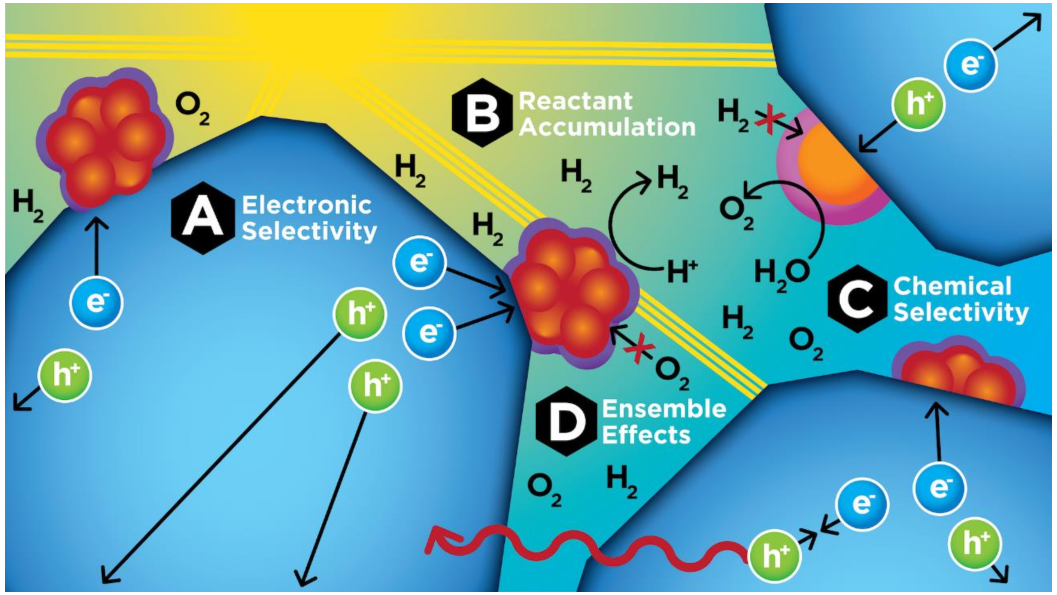
https://efrc.uark.edu/

University of Arkansas · The George Washington University, Washington, DC · Dartmouth · Berkeley University of California · University of Delaware · Rensselaer · ASU · UAPB

µ ATOMS

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, *via concerted efforts spanning the four research thrusts of (A) Electronic Selectivity, (B) Reactant Accumulation, (C) Chemical Selectivity, and (D) Ensemble Effects*.

RESEARCH PLAN

EPN strives to advance the frontiers of discovery in solar photochemical fuel formation, recognizing that sunlight generates diffuse electronic charges, yet these charges must be concentrated to form the energy-dense chemical bonds in fuels. To achieve this goal, EPN aims to extend the lifetime of reaction intermediates, thus increasing the yields for charge separation and charge accumulation at reaction centers, while also enhancing redox selectivity, and therefore stability, that together dictate solar energy conversion efficiencies of nanoreactor ensembles.

EPN

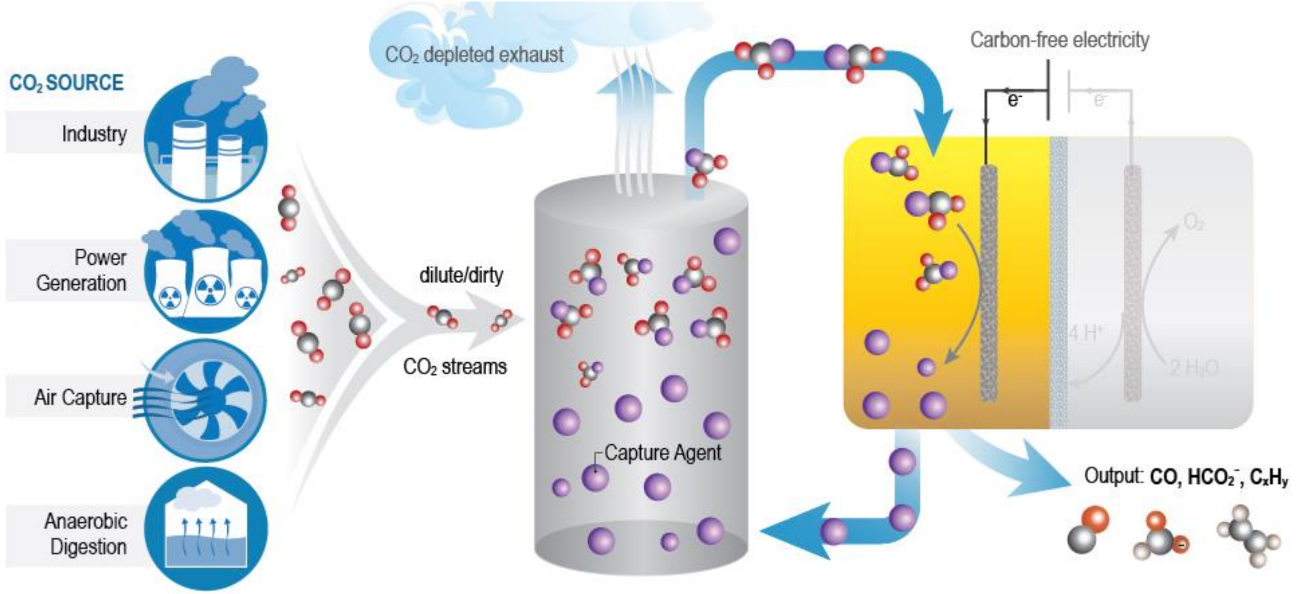
https://photosynthesis.uci.edu/

University of California, Irvine · California State University Long Beach · Colorado State University · Fort Lewis College · University of Colorado Boulder · Yale · Caltech · Sandia National Laboratories · Lawrence Livermore National Laboratory · NREL Transforming ENERGY · Columbia University in the City of New York · Medgar Evers College · University of Michigan

The Center for Closing the Carbon Cycle (4C)

Jenny 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 is advancing the foundational science and defining 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.

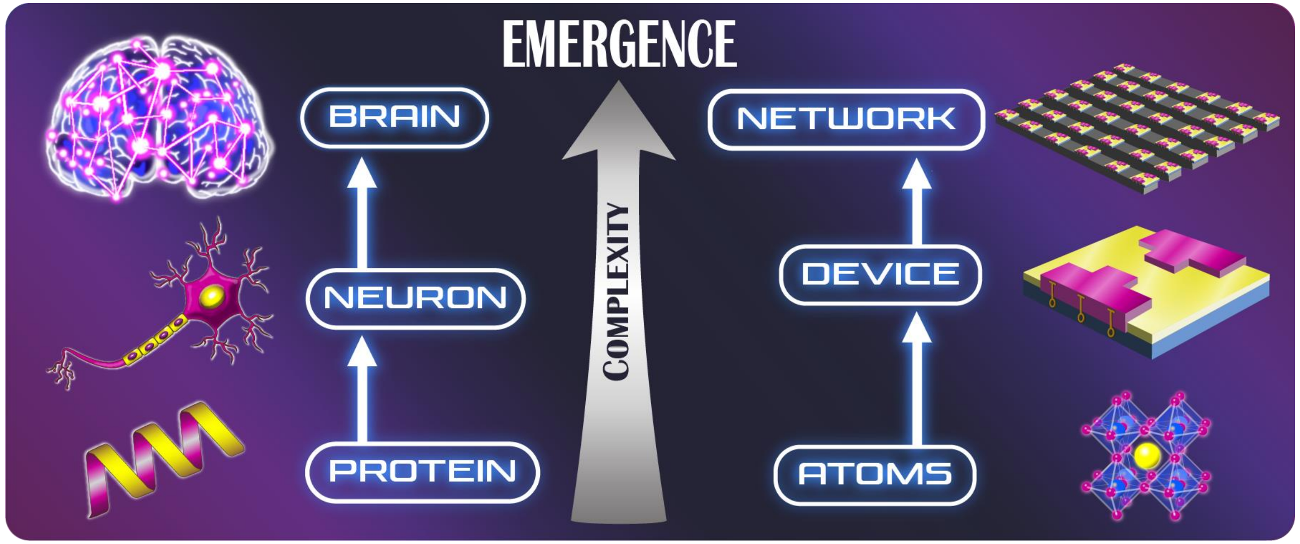
https://carbon solution.uci.edu/

UCI University of California, Irvine; University of Louisville; University of Michigan; Oak Ridge National Laboratory; University of Colorado Boulder; UC Davis; PennState; Lawrence Livermore National Laboratory; Case Western Reserve University; Caltech; CalPoly Pomona; UCLA; University of Central Arkansas; ECSU Elizabeth City State University

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”).



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

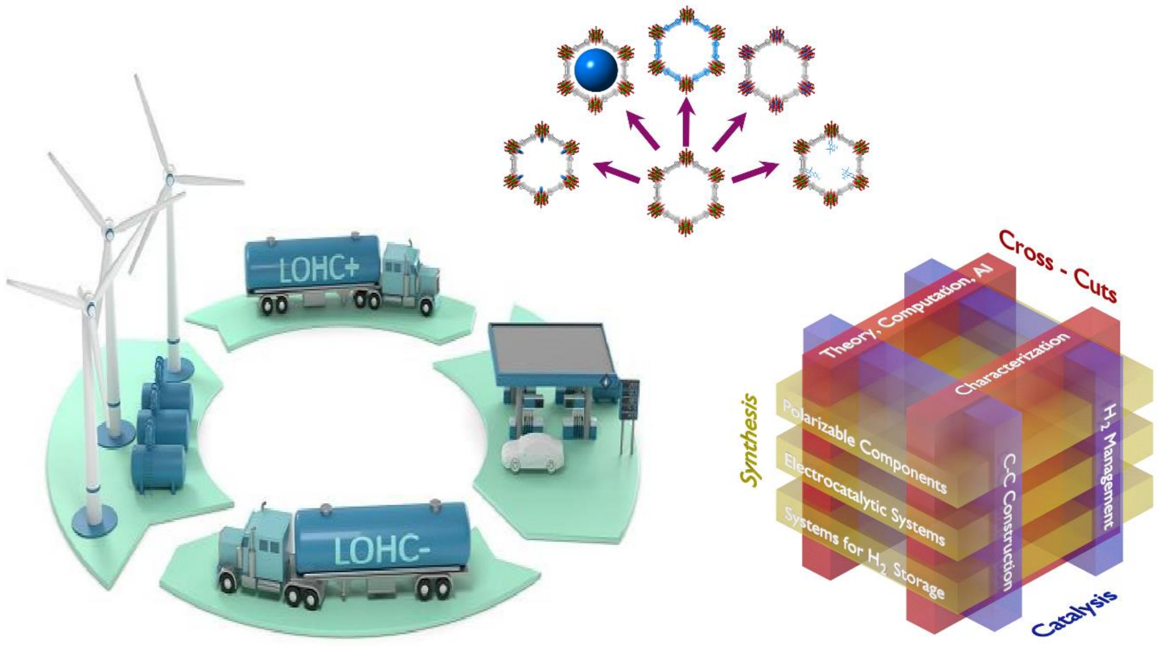
https://qmeenc.ucsd.edu/

UC San Diego | UCSB | ILLINOIS | RUTGERS | Brookhaven National Laboratory | NYU | THE UNIVERSITY OF TENNESSEE KNOXVILLE | UC DAVIS | THE UNIVERSITY OF CHICAGO

Catalyst Design for Decarbonization Center (CD4DC)

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

MISSION: Identify promising pathways for H_2 addition and removal into carbon-based energy carriers. Identify the mechanism of the required reactions experimentally and theoretically in order to guide catalyst development. Discover and develop ***reticular metal-organic framework*** materials as unique catalysts for low-temperature hydrogen addition and removal as well as carbon-carbon bond manipulation.



RESEARCH PLAN: CD4DC will address the essential need for alternate forms of H_2 transport and storage, via the development of CH_3OH and liquid organic hydrogen carriers (LOHCs), and discover new, low temperature, high activity catalysts for hydrogen addition and removal, and C-C bond formation.

https://cd4dc.center.uchicago.edu

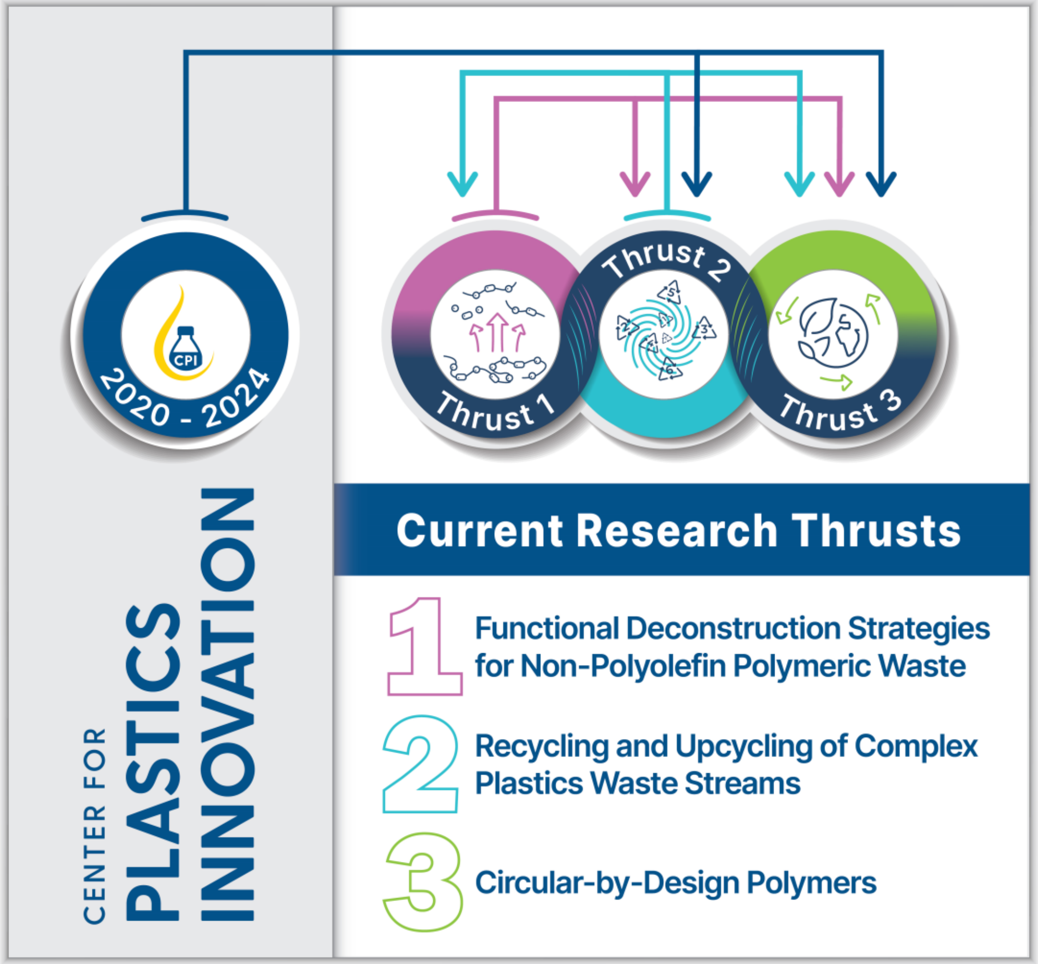
The University of Chicago · Argonne National Laboratory · Northwestern University · The Ohio State University · Pacific Northwest National Laboratory · Stony Brook University · University of Illinois Chicago · University of Minnesota

Center for Plastics Innovation (CPI)

LaShanda Korley (University of Delaware); Class: 2020-2028

MISSION: To develop energy-efficient, selective, and tolerant chemo- and bio-catalytic and synthetic pathways to valorize diverse plastics waste streams and dramatically increase circularity.

RESEARCH PLAN: CPI will deliver disruptive, transformative, and foundational solutions to realize more sustainable plastics throughout their life cycle. We explore deconstruction routes that synergize chemical and enzymatic approaches to produce building blocks from heteroatomic polymers, define pathways to enable tailored deconstruction of waste streams with compositional complexity, and employ methods to impart selective sites for degradation/improved recyclability. This research nucleates a paradigm shift in the plastics life cycle *via* detailed mechanistic understanding.



https://cpi.udel.edu

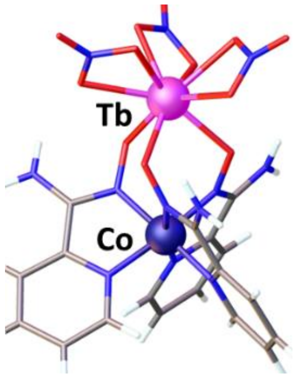
CENTER FOR PLASTICS INNOVATION · University of Delaware · The University of Chicago · Penn · Oak Ridge National Laboratory · The University of North Carolina at Chapel Hill · UF University of Florida

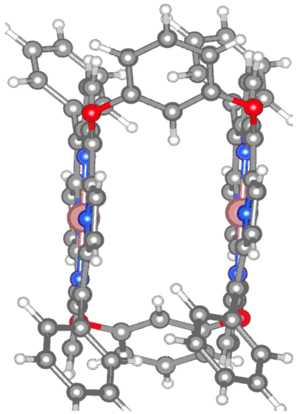
Center for Molecular Magnetic Quantum Materials(M2QM)

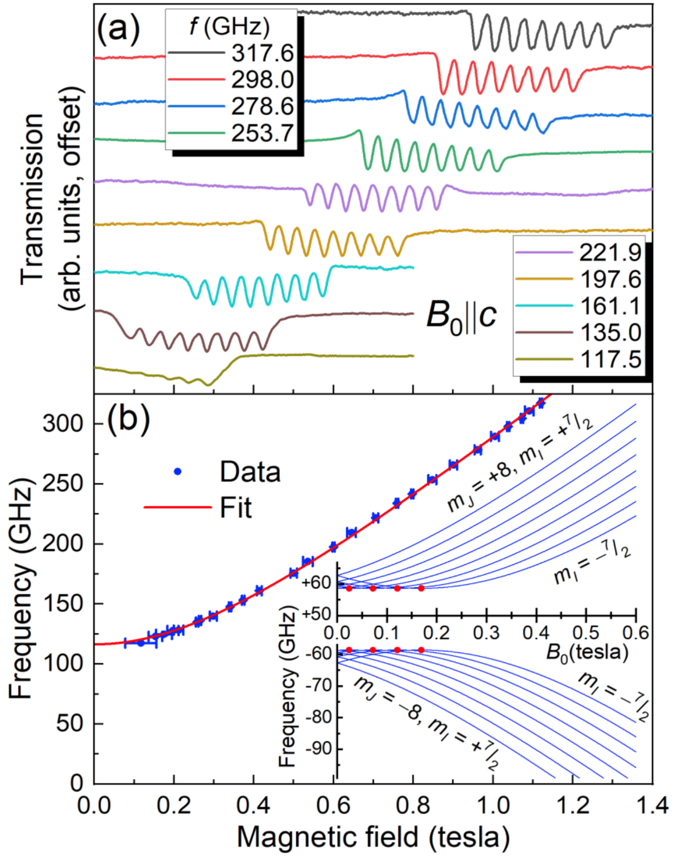
Xiaoguang Zhang (University of Florida); Class: 2018-2026

MISSION: To provide the materials physics and chemistry understanding of molecular magnetic quantum materials essential for quantum and conventional computing beyond Moore's Law.

RESEARCH PLAN: The overarching goal is to turn molecular magnets into quantum materials useful for both quantum computing and quantum current conventional devices.







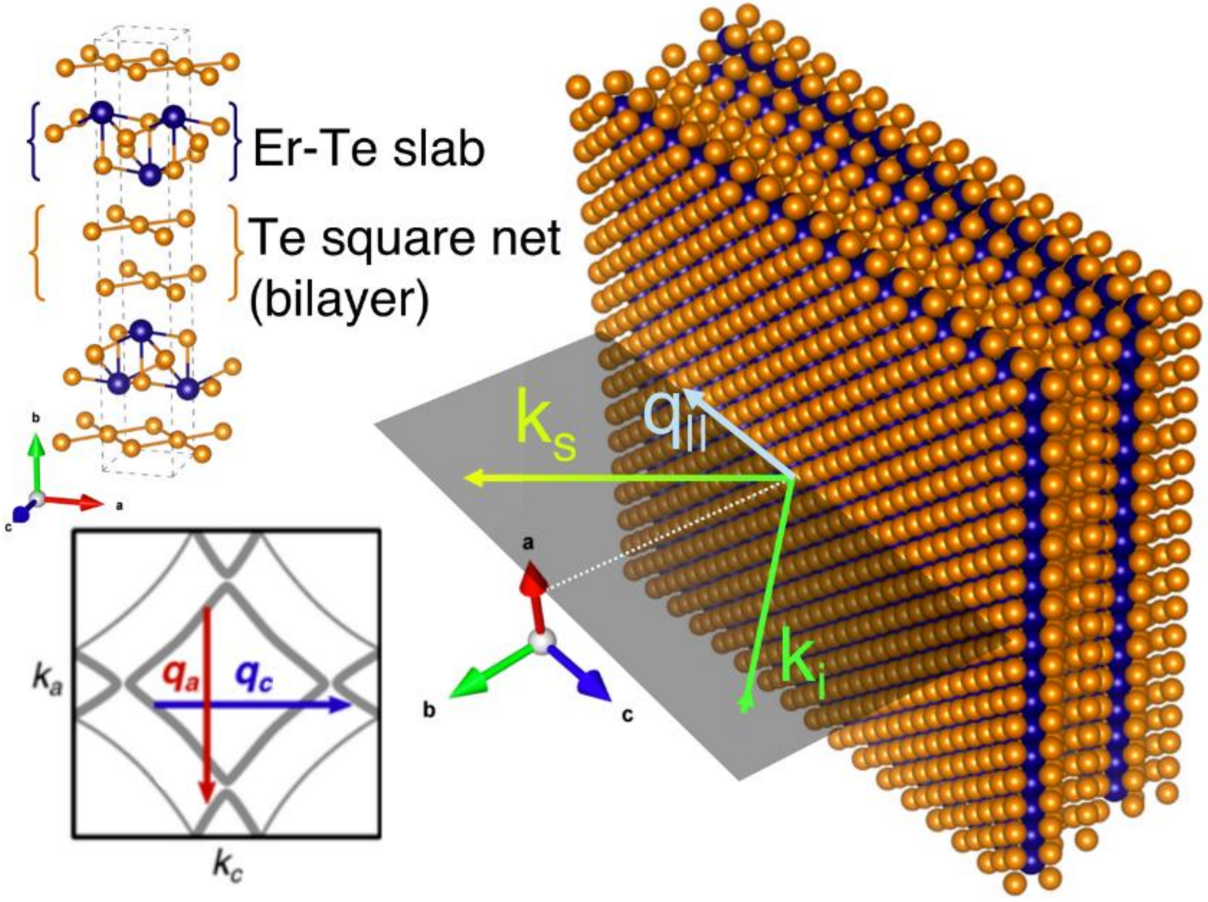
http://efrc.ufl.edu/

Quantum Sensing and Quantum Materials (QSQM)

Peter Abbamonte (University of Illinois); Class: 2020-2026

MISSION: To apply advanced scattering and scanning probe spectroscopy techniques to study charge dynamics in quantum materials.

RESEARCH PLAN: The QSQM aims to use advanced scattering and scanning probe spectroscopy techniques to measure the fundamental charge excitations in the latest generation of quantum materials, including strange metals, charge density wave materials, interacting topological phases, focusing on quantifying the degree of quantum entanglement and information density.



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

ILLINOIS Materials Research Laboratory GRAINGER COLLEGE OF ENGINEERING

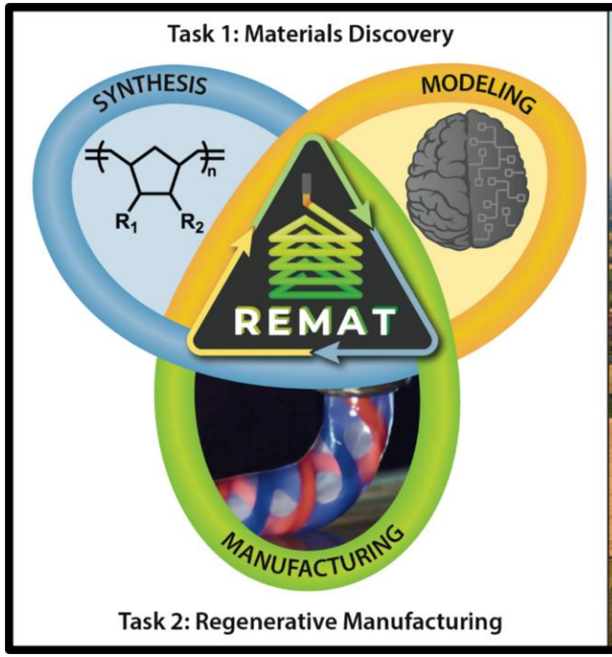
SLAC NATIONAL ACCELERATOR LABORATORY

QSQM

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.



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.

www.remat.Illinois.edu

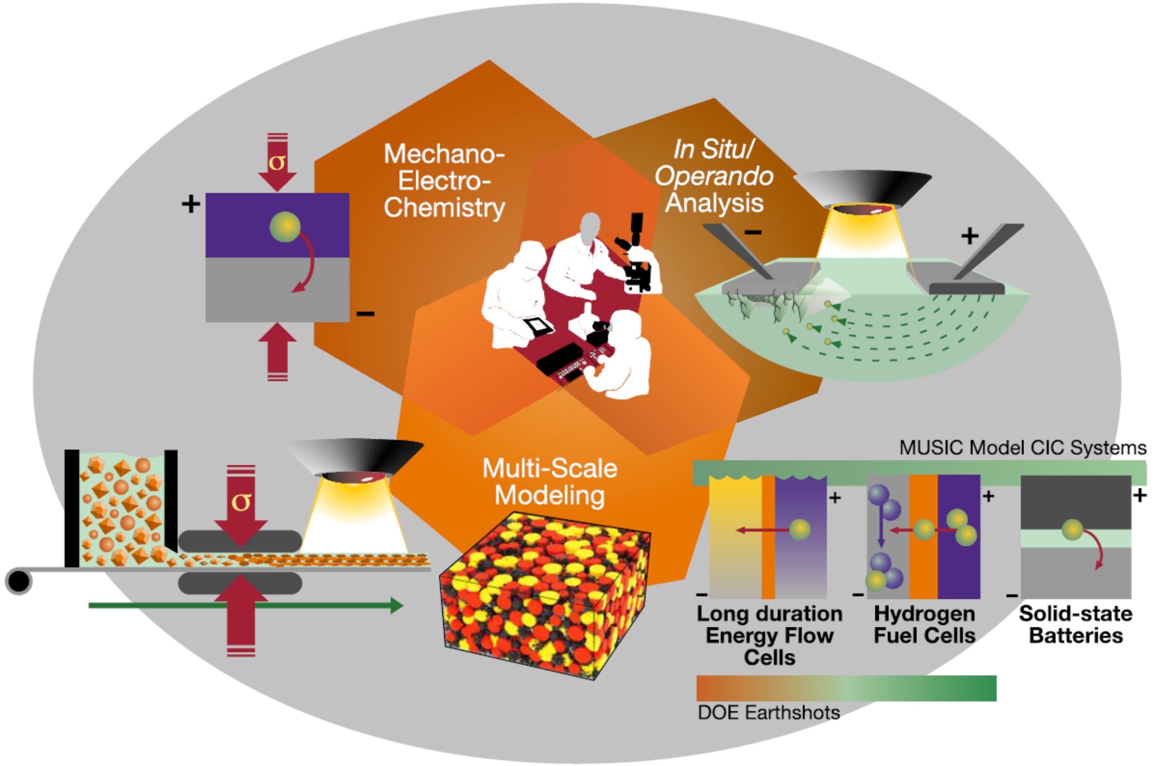
Harvard John A. Paulson School of Engineering and Applied Sciences

Sandia National Laboratories

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.



RESEARCH PLAN:

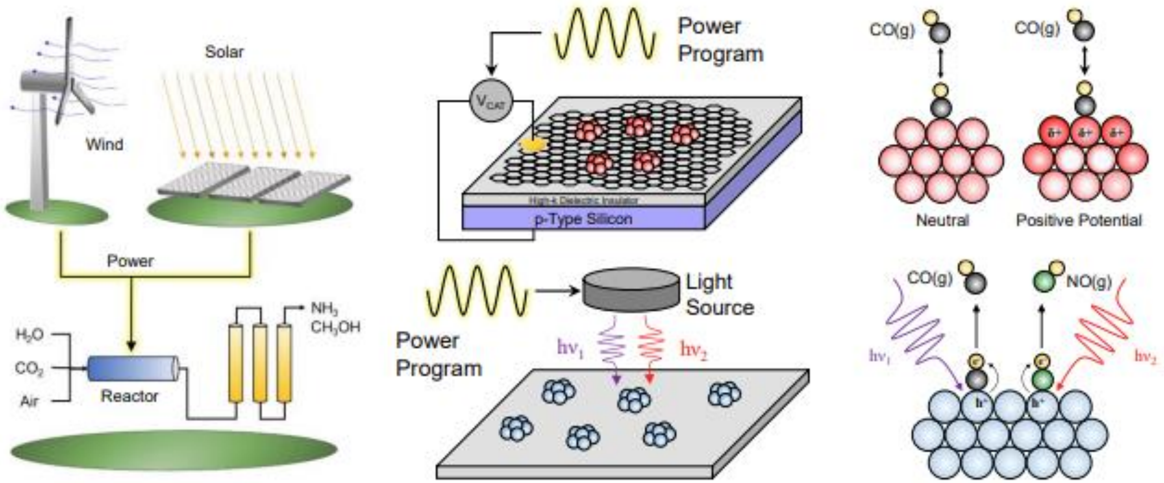
- **Thrust 1**: Revealing electrochemical-mechanical coupling at CIC interfaces and interphases
- **Thrust 2**: Understanding material degradation pathways in CIC-based electrochemical systems
- **Thrust 3**: Science of synthesis, processing, and manufacturing of CICs

https://musicefrc.engin.umich.edu/

Center for Programmable Energy Catalysis (CPEC)

Paul 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.



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.

WWW.CPEC.UMN.EDU

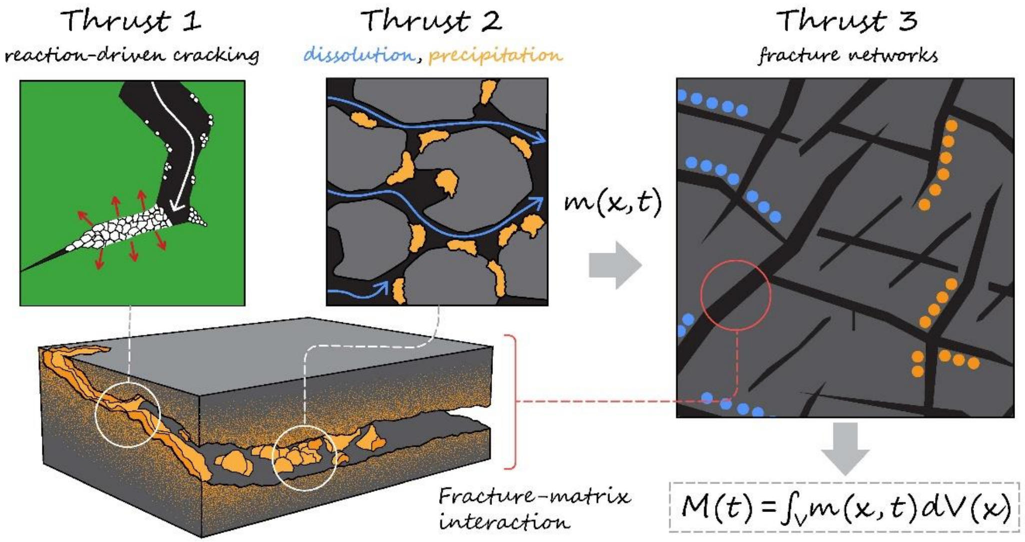
University of Minnesota | Massachusetts Institute of Technology | The Ohio State University | University of Michigan | UCSB University of California Santa Barbara | University of Houston | Center for Programmable Energy Catalysis

Geo-processes in Mineral Carbon Storage (GMCS)

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

MISSION: To develop the fundamental science that will lead to realizing the full potential for the large-scale subsurface storage of CO_2 via mineralization

RESEARCH PLAN: A promising strategy to reduce anthropogenic CO_2 is to permanently mineralize carbon in the subsurface. To allow for the engineered enhancement of this process, GMCS is closing critical knowledge gaps by: (1) identifying the coupled chemo-hydro-mechanical processes leading to the formation of microcracking in the rock matrix; (2) delineating the transport mechanisms that deliver the CO_2 charge to reactive sites; (3) establishing computational and sensing technologies that integrate this knowledge into large-scale characterization and prediction of the effectiveness of a host rock. We aim to evaluate, for a given CO_2 storage operation within a given rock mass, the evolution of the amount of carbon $M(t)$ mineralized: $M(t) = \int_V m(\mathbf{x}, t)\,\mathrm{d}V(\mathbf{x})$



***GMCS** … where geomechanics meets geochemistry in the subsurface*

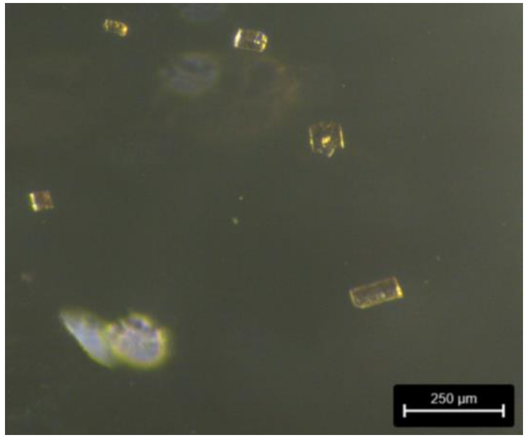
GMCS — Advancing permanent mineral storage of carbon dioxide in geologic formations

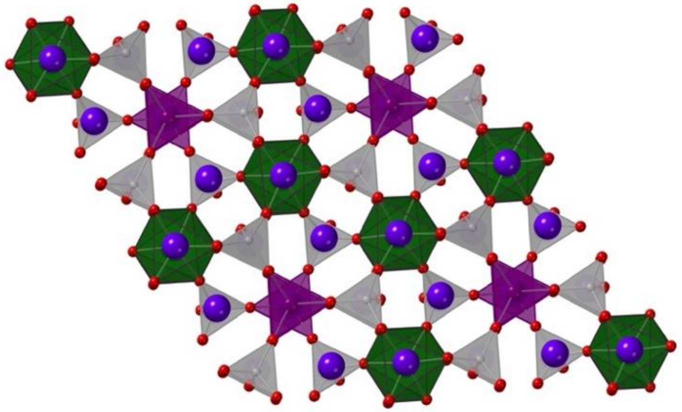
https://gmcs.umn.edu/

University of Minnesota | Georgia Institute of Technology | Los Alamos National Laboratory | Northwestern | University of Southampton

Center for Hierarchical Waste Form Materials (CHWM)
Hans-Conrad zur Loye (University of South Carolina); Class 2016-2025

MISSION: Advance an understanding of the atomic environment in extended crystalline structures and their response to radiation fields and radiolytic processes to help design and predict the behavior of novel, robust nuclear waste forms.





RESEARCH PLAN: The unique predictive and synthetic capabilities developed in the center will be used to study the crystal chemistry of transuranic (TRU) containing extended crystalline structures, to elucidate which types of structural elements favor radiation resiliency of TRU-containing extended structures, and to investigate their response to radiation damage and radiolytic processes.

https://chwm.sc.edu

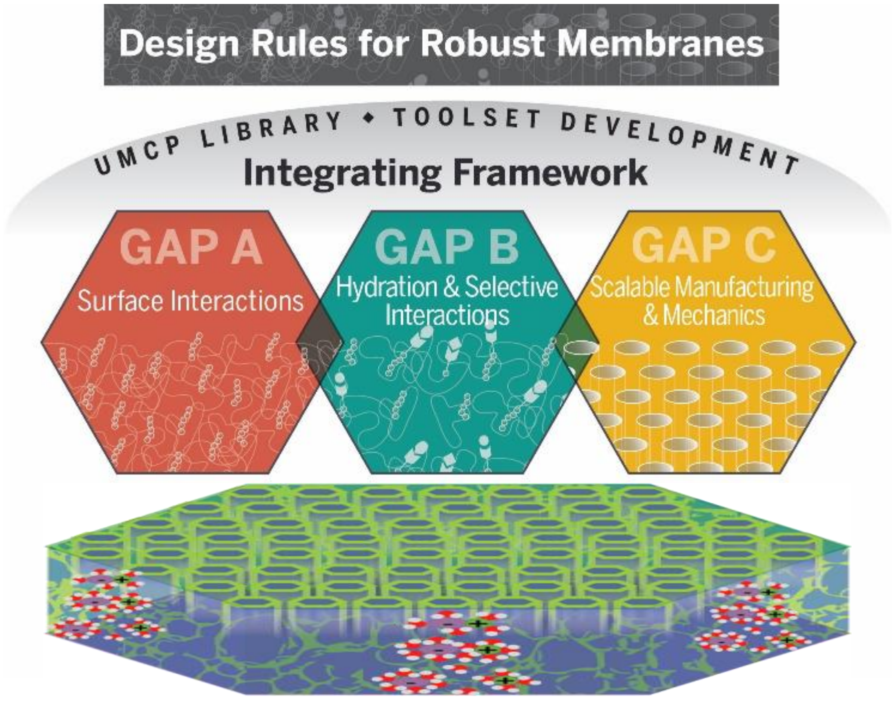
Alfred University | UofSC South Carolina | Savannah River National Laboratory | CHWM Center for Hierarchical Wasteform Materials

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.

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



https://mwet.utexas.edu/

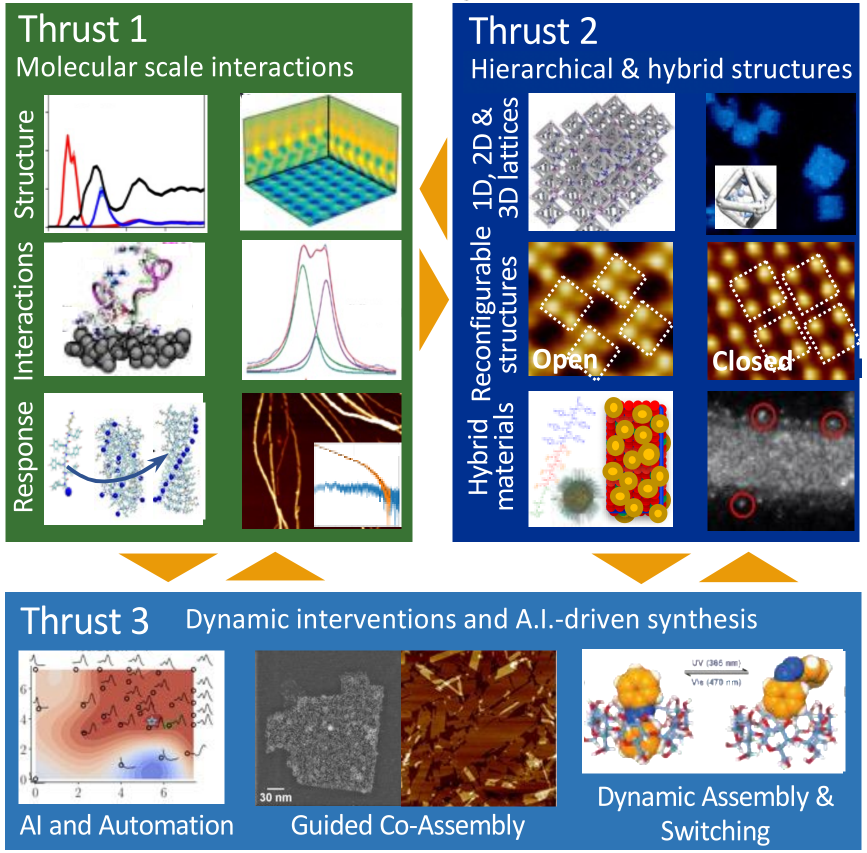
TEXAS The University of Texas at Austin | UC SANTA BARBARA | BERKELEY LAB | MWET CENTER FOR MATERIALS FOR WATER AND ENERGY SYSTEMS

Center for the Science of Synthesis Across Scales (CSSAS)

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

MISSION: 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 phases; master free energy landscapes to control their assembly into hierarchical and hybrid materials; and access new states of matter through the integration of synthesis, simulations, *in situ* characterization, data science, and AI.



https://www.cssas-efrc.com

CSSAS Center for the Science of Synthesis Across Scales · University of Washington · Pacific Northwest National Laboratory · The University of Chicago · UC San Diego · The University of Tennessee Knoxville · Columbia University · NC State University

GRAND CHALLENGES INDEX

TRANSFORMATIVE OPPORTUNITIES INDEX

BES REPORTS INDEX