U.S. Department of Energy

Energy Frontier Research Centers

One Page Overviews

Office of Science
9/19/2020

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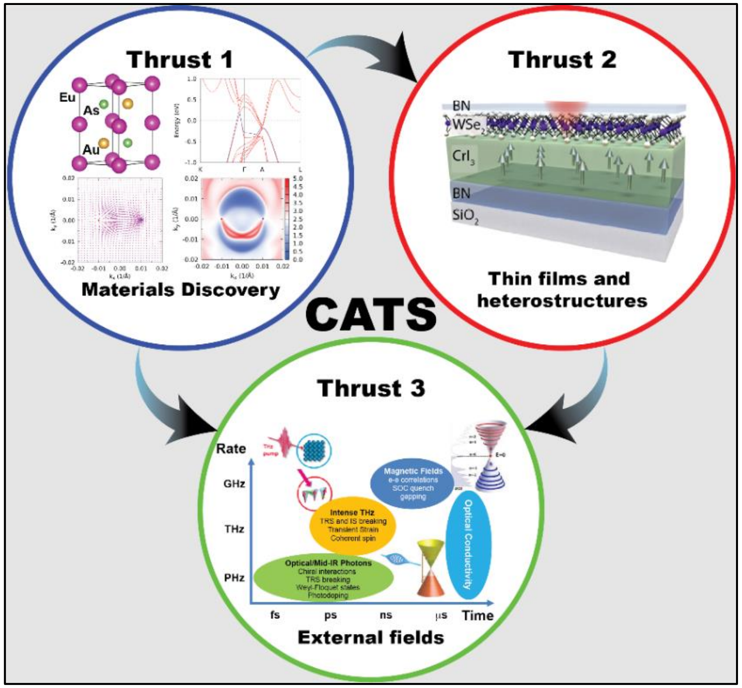
Ordered by Institution and then by Director

Center for the Advancement of Topological Semimetals (CATS)

Robert McQueeney (Ames Laboratory); Class: 2018-2022

MISSION: To discover and understand new magnetic topological materials that host quantum phenomena and functionality for future applications in computing, spin-based electronics, and sensing.



https://cats.ameslab.gov

RESEARCH PLAN

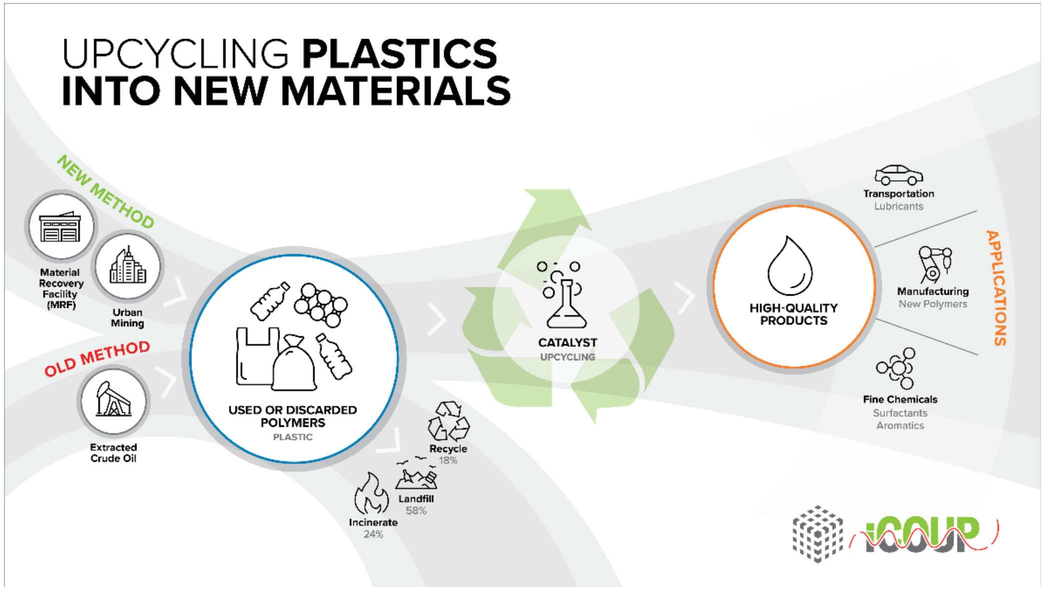
CATS has crosscutting research thrusts to; (1) predict, discover, and understand new magnetic topological materials, (2) discover and control novel quantum states and functionality in thin films and heterostructures, and (3) investigate the manipulation of topological states with external fields.

U.S. DEPARTMENT OF ENERGY | Office of Science | CATS | AMES LABORATORY | Argonne NATIONAL LABORATORY | HARVARD UNIVERSITY | Los Alamos NATIONAL LABORATORY | Massachusetts Institute of Technology | UC SANTA BARBARA | UNIVERSITY OF WATERLOO

Institute for Cooperative Upcycling of Plastics (iCOUP)

Aaron Sadow (Ames Laboratory); Class: 2021-2024

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

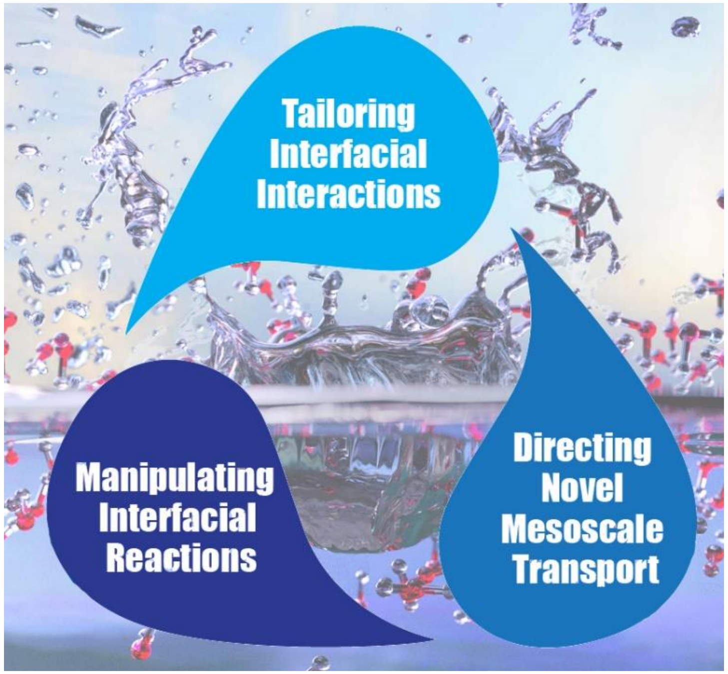
iCOUP is creating inorganic catalysts to cleave specific bonds in polyolefins, discovering new methods for polymer upcycling into value-added products and materials, and understanding the phenomena, such as macromolecule-catalyst interactions, underpinning these transformations.

U.S. DEPARTMENT OF ENERGY | Office of Science | AMES LABORATORY | Northwestern University | ILLINOIS | UCSB | Cornell University | Argonne NATIONAL LABORATORY | UNIVERSITY OF SOUTH CAROLINA | iCOUP

Advanced Materials for Energy-Water Systems (AMEWS)

Seth Darling (Argonne National Laboratory); Class: 2018-2022

MISSION: To understand and design water-solid interfaces to enable future advances in materials for efficient water treatment.



https://www.anl.gov/amews

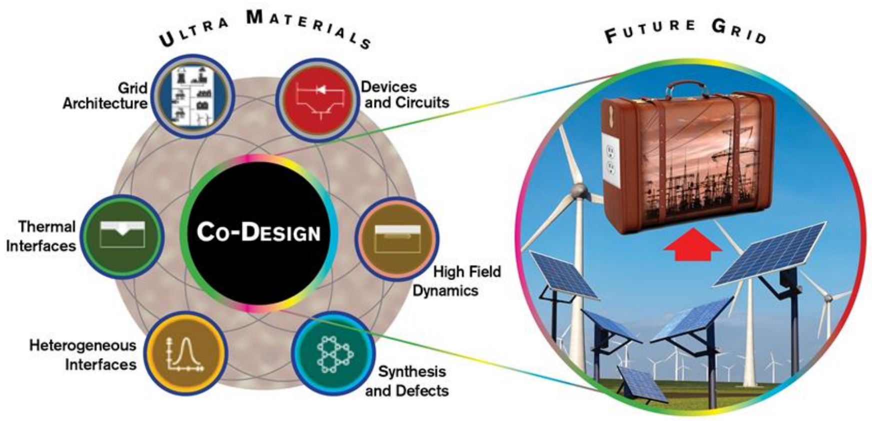
RESEARCH PLAN

AMEWS combines experiments and theory/modeling/simulation to explore interfaces between solids and aqueous fluids to gain predictive understanding of adsorption, reactivity, and transport in energy-water systems.

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.



Website URL: TBD

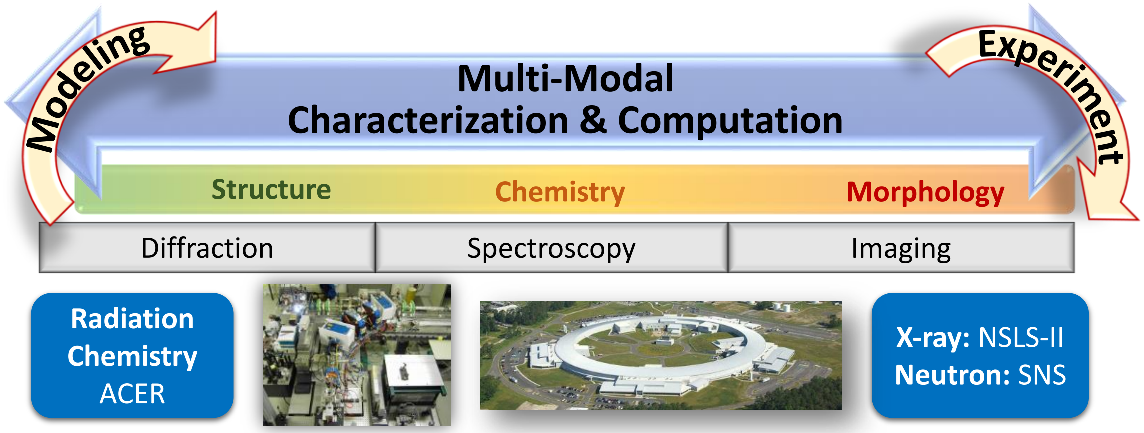
RESEARCH PLAN:

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: 2018-2022

MISSION: To provide a fundamental under-standing of the bulk and interfacial chemistry of molten salts that will underpin molten salt reactor technology.



https://www.bnl.gov/moltensalts/

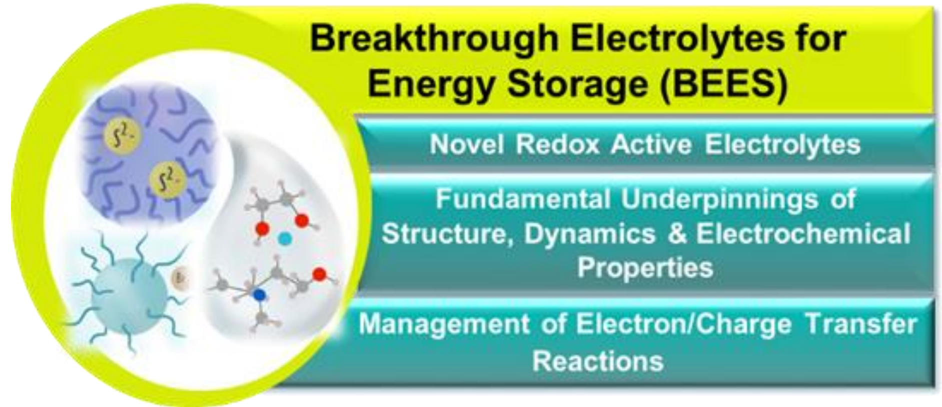
RESEARCH PLAN

Coordinated experimental and theoretical efforts using cutting-edge capabilities at DOE-SC User Facilities and at partner institutions as well as high-performance computing will examine the atomic basis of molten salt behavior under the coupled extremes of high temperature and ionizing radiation to provide a predictive description of molten salt chemistry.

Breakthrough Electrolytes for Energy Storage (BEES)

Robert Savinell (Case Western Reserve University); Class: 2018-2022

MISSION: To develop a fundamental understanding of: (i) solvation and transport properties; (ii) electrode-electrolyte interfaces; and (iii) electron transfer reactions in deep eutectic solvents and soft nanoparticle electrolytes.



https://engineering.case.edu/EFRC BEES

RESEARCH PLAN

Synergizing experimental and theoretical investigations, BEES researchers employ electroanalytical techniques, spectroscopy, synchrotron based X-ray and neutron techniques, as well as advanced computational methods to probe structures, fundamental properties, and interfacial chemistry. This fundamental know-how will enable design and synthesis of new electrolytes that will transform energy storage.

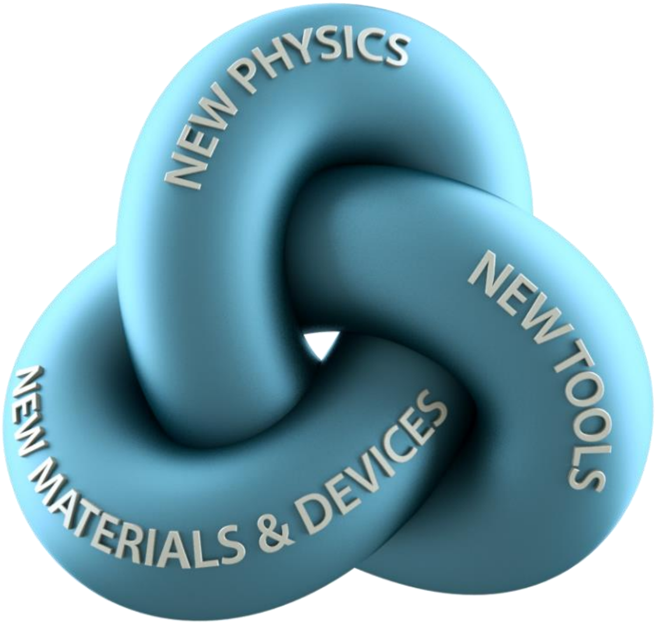
U.S. DEPARTMENT OF ENERGY | Office of Science

Case Western Reserve University · The University of Tennessee · NYU · Hunter, The City University of New York · Texas, The University of Texas at Austin · Columbia University · University of Notre Dame · Brookhaven National Laboratory · Texas A&M University

Programmable Quantum Materials (Pro-QM)

Dmitri N. Basov (Columbia University); Class: 2018-2022

MISSION: To discover, characterize, and deploy new forms of quantum matter controllable by gating, magnetic proximity and nano-mechanical manipulation.



https://quantum-materials.columbia.edu

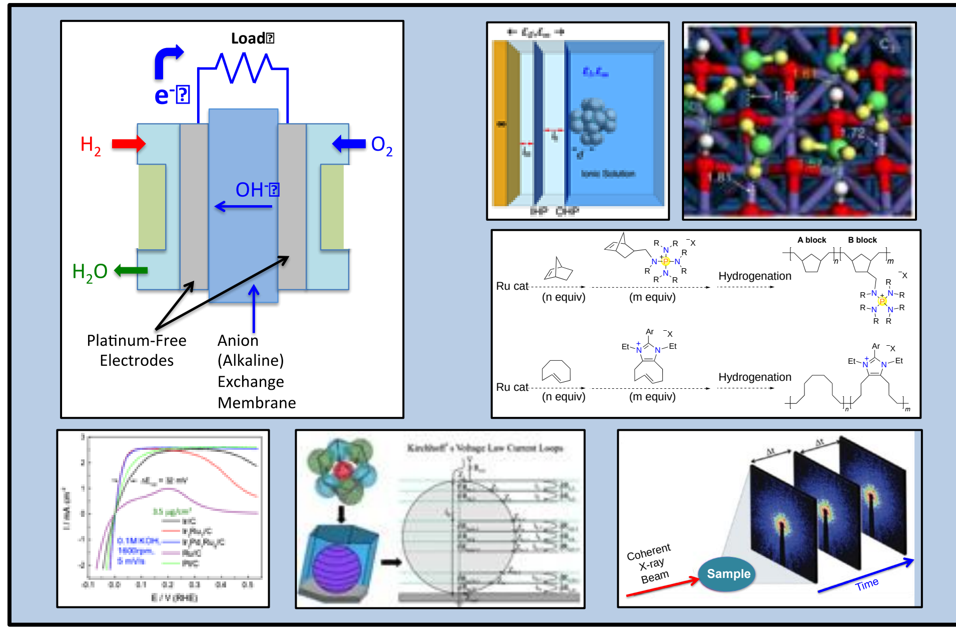
RESEARCH PLAN

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

Center for Alkaline Based Energy Solutions (CABES)

Héctor D. Abruña (Cornell University); Class: 2018-2022

MISSION: To achieve a detailed understanding of the nature, structure, and dynamics of electrocatalysis in alkaline media.



https://cabes.cornell.edu/

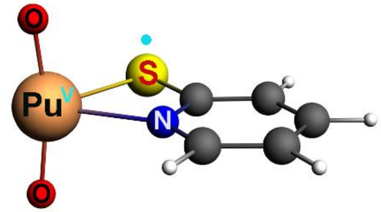
RESEARCH PLAN

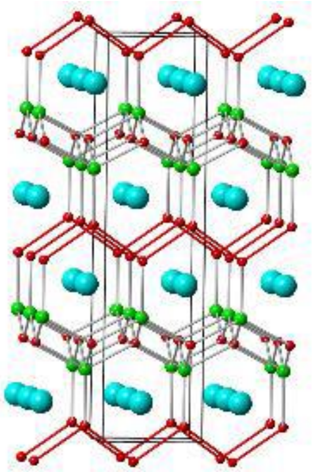
CABES seeks a detailed understanding of the nature, structure, and dynamics of fuel cell systems operating in alkaline media. The center will integrate theory and computational methods, synthesis of electrocatalysts and novel membrane materials, and the development of experimental tools that will provide in situ, spatiotemporal characterization of systems under operation.

Center for Actinide Science & Technology (CAST)

Thomas E. Albrecht-Schoenzart (Florida State University); Class: 2016-2022

MISSION: To advance our understanding of how electronic structure and bonding control the properties of radioactive materials. This knowledge will aid in the development of nuclear technologies that enhance energy security, address nuclear legacy issues, and foster the next generation of nuclear scientists.





https://cast.magnet.fsu.edu/

RESEARCH PLAN

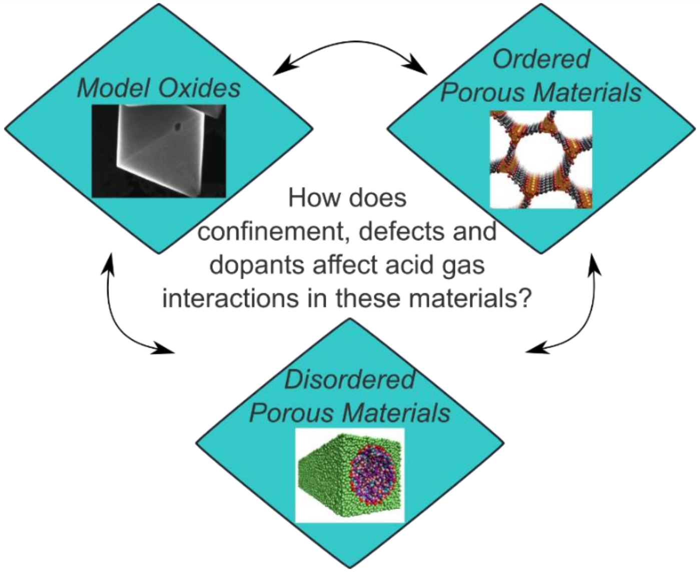
CAST develops new materials that capture radionuclides found within legacy waste from the Cold War. Optimization of these materials requires advances in synthesis, characterization, and theory that provide a deep understanding of the origin of the unusual properties of these nuclear materials.

U.S. DEPARTMENT OF ENERGY | Office of Science

Center for Understanding and Control of Acid Gas-Induced Evolution of Materials for Energy (UNCAGE-ME)

Ryan Lively (Georgia Tech); Class: 2014-2022

MISSION: To develop and harness a deep knowledge base in the characterization, prediction, and control of acid-gas interactions with a broad class of materials to accelerate materials discovery in acid gas separations, conversion, and utilization.



https://efrc.gatech.edu

RESEARCH PLAN

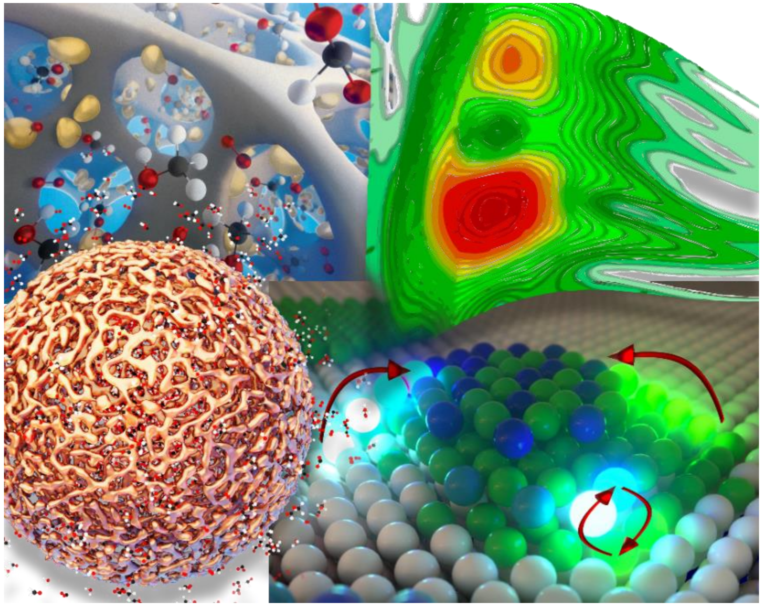
Degradation effects are often decisive factors in the practical use of materials such as sorbents for carbon capture, acid gas conversion, and natural gas purification. UNCAGE-ME's core research model is to use a variety of in-situ experimental tools coupled with complimentary modeling techniques and machine learning to improve the performance of materials in these environments and ultimately advance materials discovery.

U.S. DEPARTMENT OF ENERGY | Office of Science | Georgia Institute of Technology | Oak Ridge National Laboratory | The University of Alabama | Sandia National Laboratories | PennState | Lehigh University | Wisconsin University of Wisconsin-Madison | Washington University in St. Louis | UNCAGE-ME

Integrated Mesoscale Architectures for Sustainable Catalysis (IMASC)

Cynthia Friend (Harvard University); Class: 2014-2022

MISSION: To establish design principles for highly selective catalytic transformations driven by dilute alloys.



https://efrc.harvard.edu/

RESEARCH PLAN

- Design and synthesize robust nanoporous dilute alloy catalysts.
- Predict catalytic selectivity by understanding kinetics and mechanism.
- Exploit rearrangement at interfaces to enhance selectivity and activity.
- Advance methodology for catalytic design.

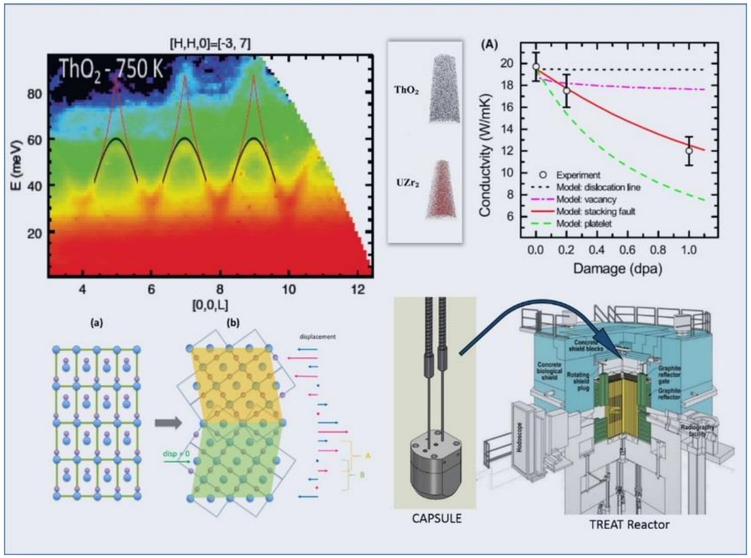
U.S. DEPARTMENT OF ENERGY | Office of Science | Harvard | Lawrence Livermore National Laboratory | Tufts University | Stony Brook University | UCLA | Penn | UF University of Florida | Brookhaven National Laboratory | Tulane University | IMASC

Center for Thermal Energy Transport under Irradiation (TETI)

David Hurley (Idaho National Laboratory); Class: 2018-2022

MISSION: To provide the foundational work necessary to accurately model and ultimately control electron- and phonon-mediated thermal transport in 5f electron materials in extreme irradiation environments.

Energy Carriers to Mesoscale Transport



https://teti.inl.gov/

RESEARCH PLAN

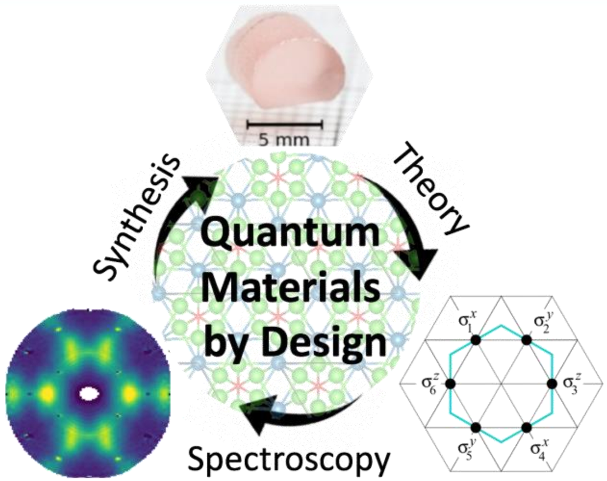
Thermal energy transport under irradiation is directly related to reactor efficiency as well as reactor safety. The aim of TETI is to develop a first principles understanding of electron and phonon transport in advanced nuclear fuels that will provide the necessary tools to enhance thermal transport by tailoring defects and microstructure.

U.S. DEPARTMENT OF ENERGY | Office of Science | INL Idaho National Laboratory | Oak Ridge National Laboratory | Purdue University | AFRL | The Ohio State University | University of Central Florida | Columbia University | TETI

Institute for Quantum Matter (IQM)

Collin Broholm (Johns Hopkins University); Class: 2018-2022

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



https://iqm.jhu.edu

RESEARCH PLAN

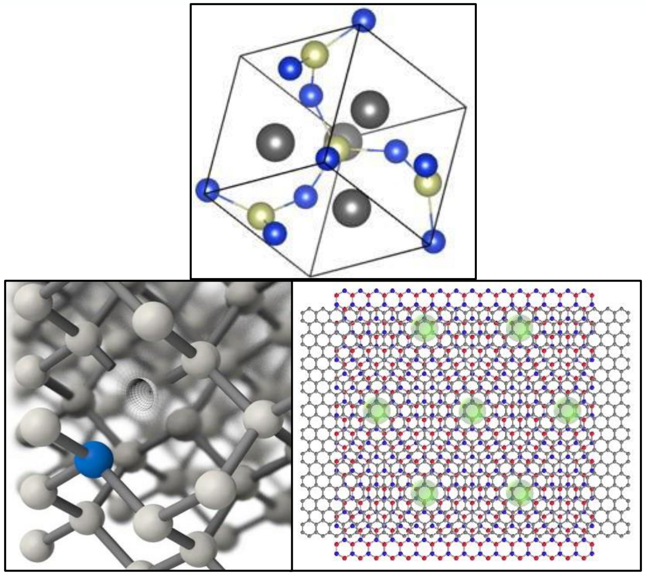
Quantum mechanics successfully describes electrons within atoms as matter waves. IQM will develop “Quantum Materials” where electronic matter waves extend beyond the atomic scale and give rise to unique physical properties. IQM theorists will identify candidate materials and nanoscale structures that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

U.S. DEPARTMENT OF ENERGY | Office of Science | JOHNS HOPKINS UNIVERSITY | Cornell University | PennState | PRINCETON UNIVERSITY | RUTGERS

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

Joel Moore (Lawrence Berkeley National Laboratory); Class: 2018-2022

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.



https://npqc.lbl.gov

RESEARCH PLAN

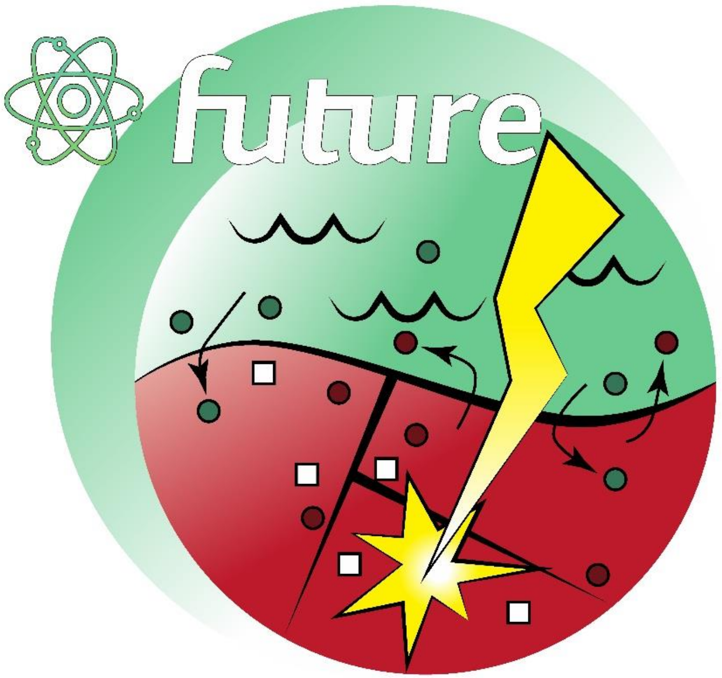
NPQC will study three families of materials in which quantum coherence is especially important, using a variety of advanced characterization techniques and theoretical methods. Major outcomes will include new approaches to solid-state quantum sensing and quantum spectroscopy, along with controllable crossovers between coherent and incoherent behavior in transport and optical properties.

U.S. DEPARTMENT OF ENERGY | Office of Science | Columbia University | UCSB | Argonne National Laboratory | Berkeley Lab | npqc

Fundamental Understanding of Transport Under Reactor Extremes (FUTURE)

Blas Pedro Uberuaga (Los Alamos National Laboratory); Class: 2018-2022

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



https://future.lanl.gov/

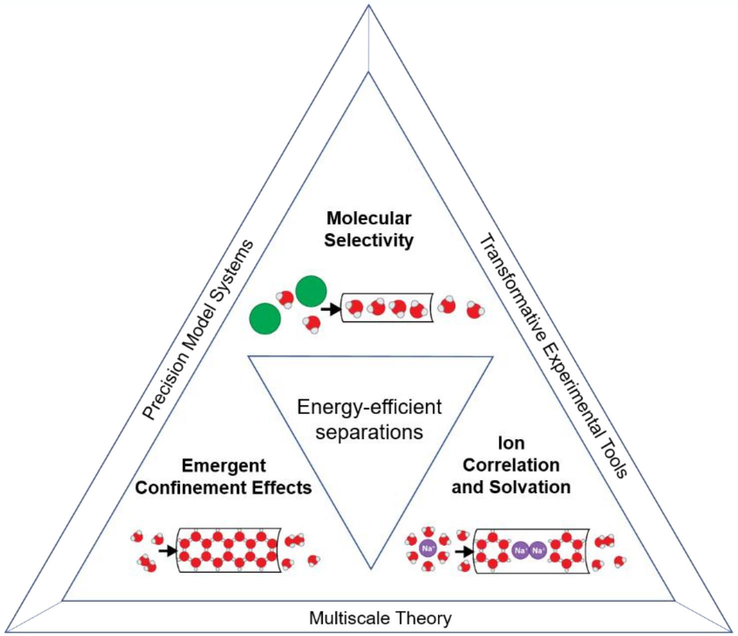
RESEARCH PLAN

FUTURE combines experiment and modeling to understand the fundamental processes responsible for materials evolution under concurrent irradiation and corrosion. The focus is on point defect production, coupled transport of chemical species in the material, and reactions at and across interfaces.

Center for Enhanced Nanofluidic Transport (CENT)

Michael Strano (MIT); Class: 2018-2022

MISSION: To address emerging and compelling gaps in our knowledge of fluid flow and molecular transport in single digit nanopores and establish the scientific foundation for developing transformative molecular separation technologies impacting the Water-Energy Nexus.



https://cent.mit.edu/

RESEARCH PLAN

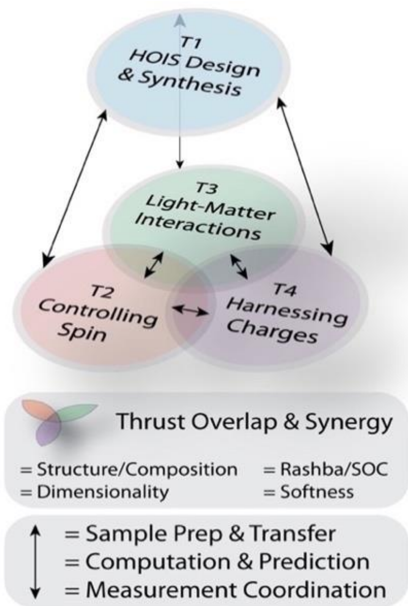
CENT will apply precision model systems, transformative experimental tools, and predictive multiscale theories to understand fluid flow and molecular transport in single-digit nanopores, to identify conditions for enhanced flow at extreme confinement, to unravel structure of solid/liquid interfaces,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

Center for Hybrid Organic Inorganic Semiconductors for Energy (CHOISE)

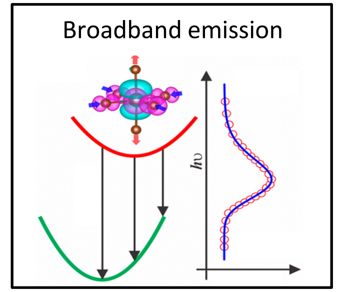
Matthew C. Beard (National Renewable Energy Laboratory); Class: 2018-2022

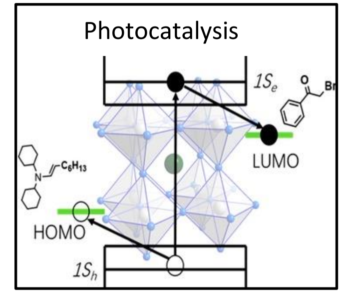
MISSION: To enable unprecedented synthetic control over the emergent phenomena of spin, charge, and light-matter interactions, in tailored organic-inorganic perovskite-inspired systems for energy science.

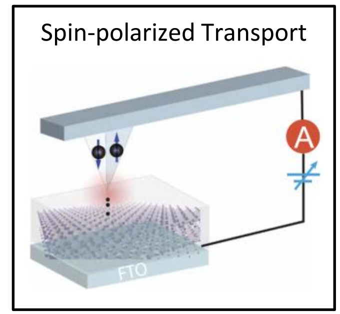
CHOISE Plan:

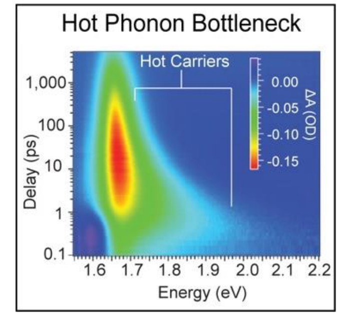


Example emergent phenomena









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

RESEARCH PLAN

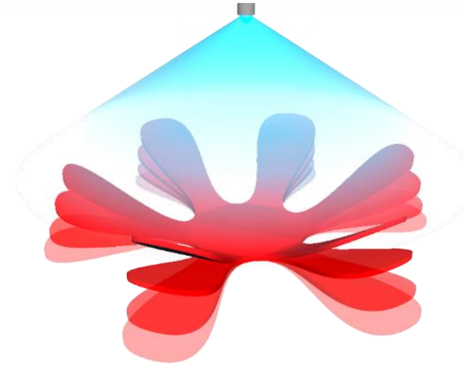
CHOISE will employ the full flexibility of organic and inorganic chemistry to design and demonstrate HOIS with unique and controllable spin, electronic, and optical properties. Key structural parameters will include metal selection, halide/psuedohalide choice, overall stoichiometry, and organic cation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

U.S. DEPARTMENT OF ENERGY | Office of Science | CHOISE Center for Hybrid Organic Inorganic Semiconductors for Energy | NREL National Renewable Energy Laboratory | Duke University | The University of Utah | Toledo | San Diego State University | The University of Chicago | University of Colorado Boulder | The University of North Carolina at Chapel Hill

Center for Bio-Inspired Energy Science (CBES)

Samuel I. Stupp (Northwestern University); Class: 2009-2022

MISSION: To develop the next frontier in soft materials relevant to energy challenges by designing structures that emulate functions we see in biological systems.



https://cbes.northwestern.edu

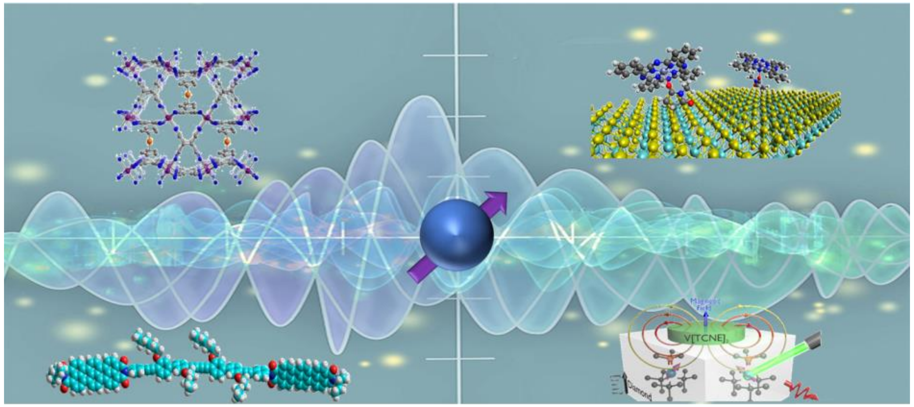
RESEARCH PLAN

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". 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 University); Class: 2020-2024

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



https://cmqt.org

RESEARCH PLAN

Quantum-to-quantum transduction is the coherent exchange of information between quantum systems, which is an essential element of quantum information science.

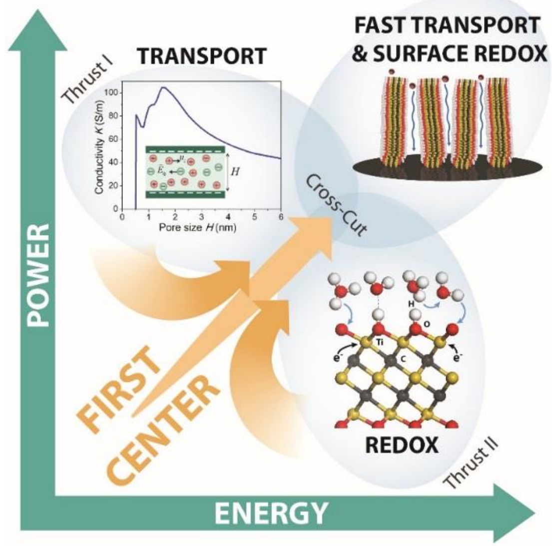
- **CMQT** explores coherent coupling of molecular degrees of freedom, i.e. the pairwise interactions between photons, excitons, magnons, phonons, spins, and charges, at both the ensemble and single-molecule levels.
- **CMQT** probes quantum transduction within distributed molecular quantum systems, 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.

U.S. DEPARTMENT OF ENERGY | Office of Science | CMQT CENTER FOR MOLECULAR QUANTUM TRANSDUCTION | Northwestern | Cornell University | IOWA | THE OHIO STATE UNIVERSITY | UC San Diego | PRINCETON UNIVERSITY | Berkeley UNIVERSITY OF CALIFORNIA | WISCONSIN UNIVERSITY OF WISCONSIN-MADISON

Fluid Interface Reactions, Structures and Transport (FIRST)

Sheng Dai (Oak Ridge National Laboratory); Class: 2009-2022

MISSION: To achieve fundamental understanding and validated, predictive models of the atomistic origins of electrolyte and coupled electron transport under nanoconfinement that will enable transformative advances in capacitive electrical energy storage and other energy-relevant interfacial systems.



www.ornl.gov/sci/first/

RESEARCH PLAN:

Thrust I integrates novel experimental and computational approaches to determine how electrolyte *transport* is affected by composition, nanoconfinement and surface chemistry/charge. Thrust II considers how fast surface *redox* reactions proceed in pseudocapacitive electrode/electrolyte systems. The Cross-Cutting Theme uses these fundamental insights to achieve *simultaneous* high power and energy density.

Center for Performance and Design of Nuclear Waste Forms and Containers (WastePD)

Gerald Frankel (Ohio State University); Class: 2016-2022

MISSION: To understand the fundamental mechanisms of waste form performance, and apply that understanding to develop design approaches for new waste forms with improved and predictable performance.

https://efrc.osu.edu

RESEARCH PLAN

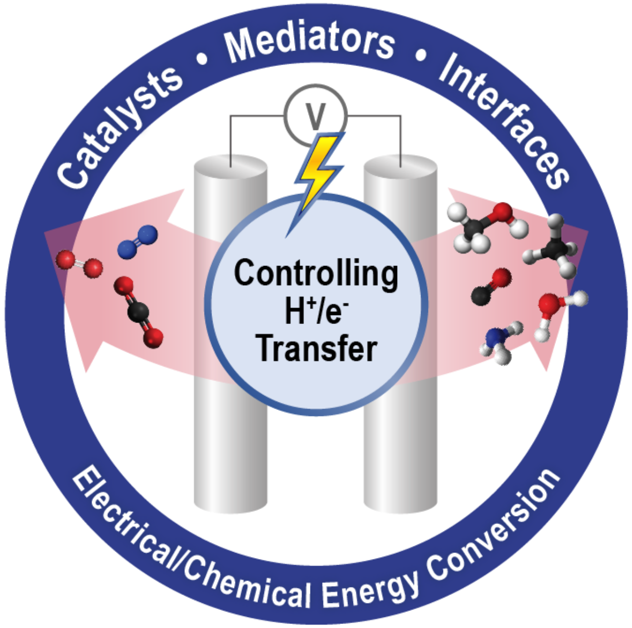
WastePD is studying the mechanisms of corrosion of glass, ceramic and metallic waste forms and containers and developing the underlying science required to design materials with improved properties and to accurately predict long term performance.

U.S. DEPARTMENT OF ENERGY | Office of Science | The Ohio State University | cea | LSU | Pacific Northwest National Laboratory | PennState | RPI | University of Virginia | QuesTek Innovations LLC | CITRINE | UNT

Center for Molecular Electrocatalysis (CME)

Morris Bullock (Pacific Northwest National Laboratory); 2009-2022

MISSION: To establish the fundamental principles needed for efficient interconversion of electrical energy and chemical bonds through precise control of electron and proton transfers.



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

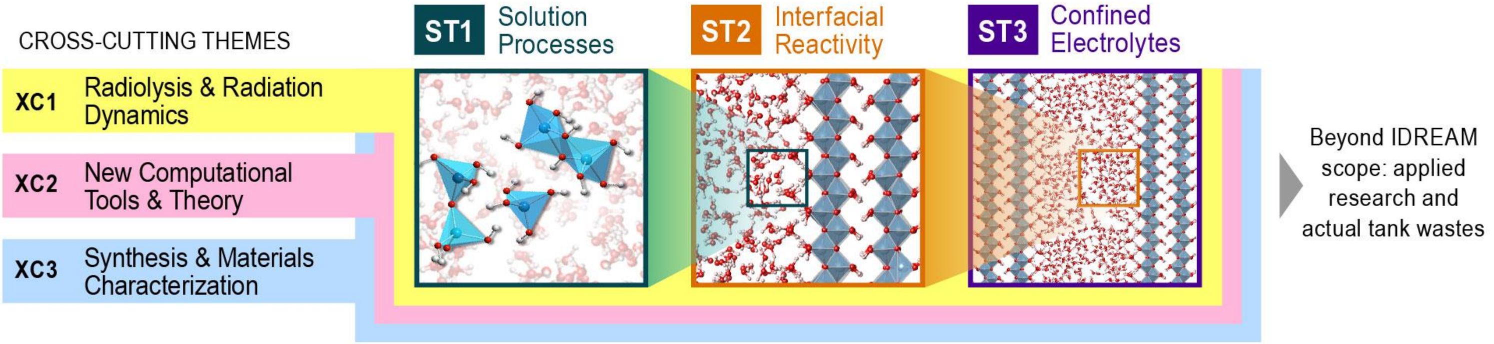
RESEARCH PLAN

CME targets fundamental discoveries in molecular electrocatalysis and interfacial reactivity to achieve fast, energy-efficient interconversion of electrical and chemical energy. CME's approach to the design of electrocatalysts exploits the emerging area of electron-proton transfer mediators and takes a molecular approach to heterogeneous interfaces.

Interfacial Dynamics in Radioactive Environments and Materials (IDREAM)

Sue Clark (PNNL); Class: 2016-2024

MISSION: To master interfacial chemistry in complex environments characterized by extremes in alkalinity and low-water activity, where molecular phenomena are driven far from equilibrium by ionizing radiation.



https://www.pnnl.gov/projects/interfacial-dynamics-radioactive-environments-and-materials

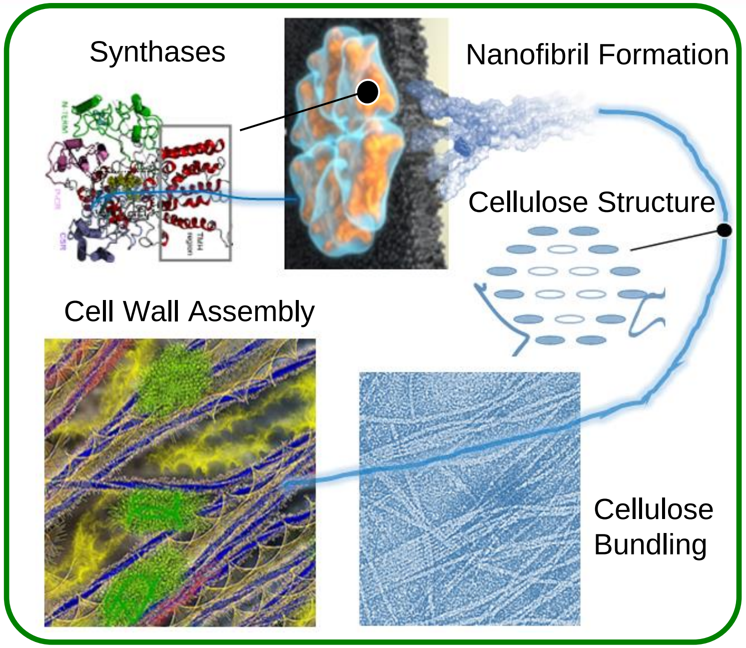
RESEARCH PLAN

IDREAM is revealing the chemical driving forces for ion behavior in alkaline electrolytes at interfaces exposed to ionizing radiation. Experimental and computational studies are integrated to discover the roles of ion networks and long-range solvent structure in solution and interfacial reactivity.

Center for Lignocellulose Structure and Formation (CLSF)

Daniel J. Cosgrove (Penn State University); Class: 2009-2022

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

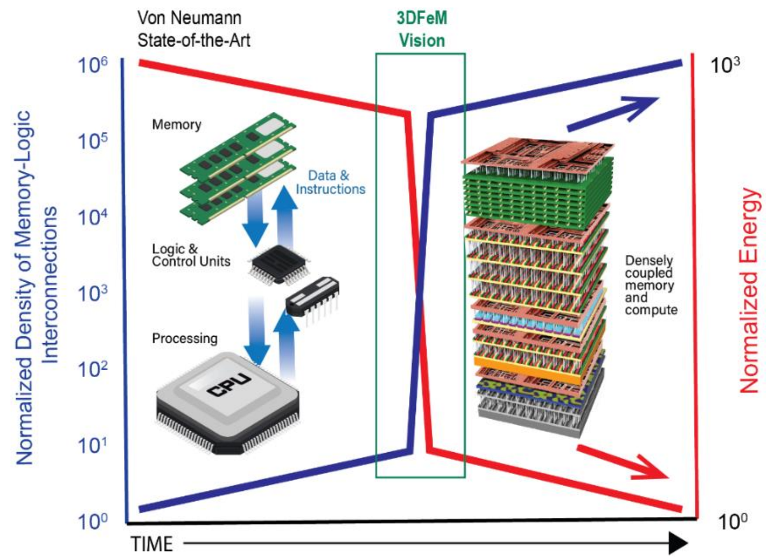
RESEARCH PLAN

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.

Three-Dimensional Ferroelectric Microelectronics (3DFeM)

Susan Trolier-McKinstry (Penn State); Class: 2020-2024

MISSION: To exploit the 3rd dimension in microelectronics for functions beyond interconnects by incorporating low-power, non-volatile ferroelectric memory. Ferroelectric materials and new devices will be co-designed, integrated reliably, and densely interconnected with logic to enable low-power, 3D non-von Neumann computation.



Website URL

RESEARCH PLAN

3DFeM will: (i) design ferroelectricity in new host crystal structures, (ii) tailor the coercive voltages through engineering emergent nanoscale inhomogeneity in scaled ultra-thin films, (iii) deposit ferroelectric materials with ancillary electronics at low temperatures at wafer scale, (iv) characterize materials at previously inaccessible time and length scales, and (v) demonstrate device functionality.

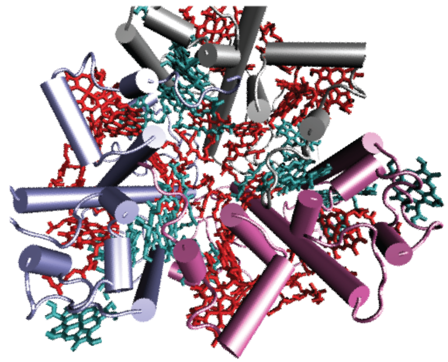
U.S. DEPARTMENT OF ENERGY | Office of Science | PennState | Purdue University | University of Virginia | Penn University of Pennsylvania | RIT Rochester Institute of Technology | Sandia National Laboratories | Oak Ridge National Laboratory

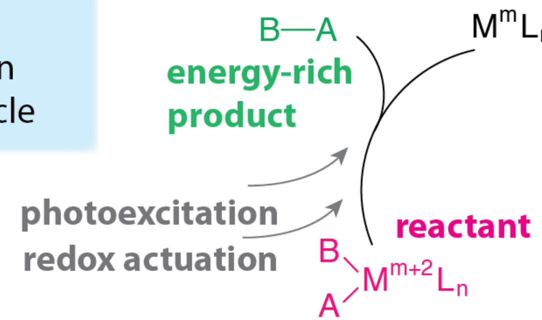
Bioinspired Light-Escalated Chemistry (BioLEC)

Gregory Scholes (Princeton University); Class: 2018-2022

MISSION: To employ light harvesting and advances in solar photochemistry to enable unprecedented photoinduced cross-coupling reactions that valorize abundant molecules.

Bioinspired multiphoton light capture & conversion empowers the catalytic cycle





Master actuation of redox states of organometallic photocatalysts by leveraging multiple photons

https://chemlabs.princeton.edu/biolec/

RESEARCH PLAN

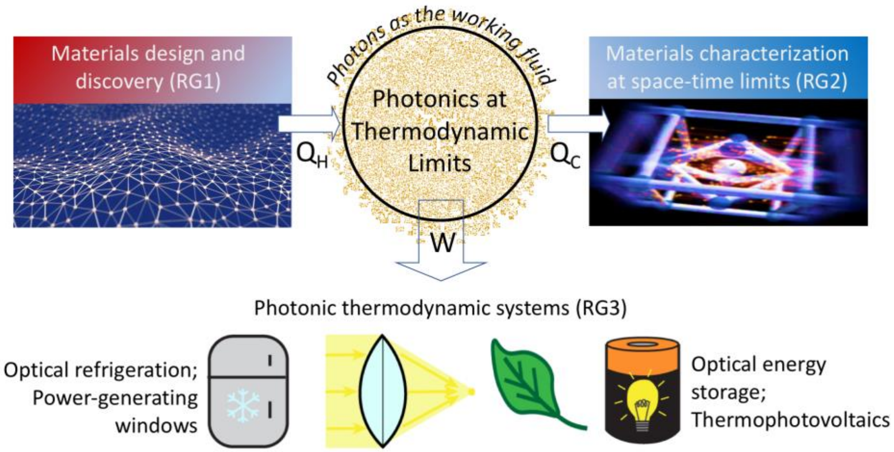
The fundamental advance of the BioLEC EFRC will be to establish a platform for directing difficult chemical transformations that are enabled by combining the energies of multiple photons. The resulting breakthroughs will yield energy-relevant chemicals, fuels, and materials.

U.S. DEPARTMENT OF ENERGY | Office of Science | PRINCETON UNIVERSITY | MICHIGAN STATE UNIVERSITY | NC STATE UNIVERSITY | MIT | Arizona State University | NREL | University of Colorado Boulder | BROOKHAVEN NATIONAL LABORATORY

Photonics at Thermodynamic Limits (PTL)

Jennifer Dionne (Stanford University); Class: 2018-2022

MISSION: To achieve photonic operations at thermodynamic limits by controlling the flow of photons, electrons, and phonons in atomically-architected materials, enabling entirely new energy conversion systems.



https://ptl.stanford.edu

RESEARCH PLAN

CHALLENGE: To design photonic conversion systems for energy and information that operate at thermodynamic limits.

APPROACH: Theory provides insights to guide materials and systems design that are in turn validated by novel, state-of-the-art characterization techniques.

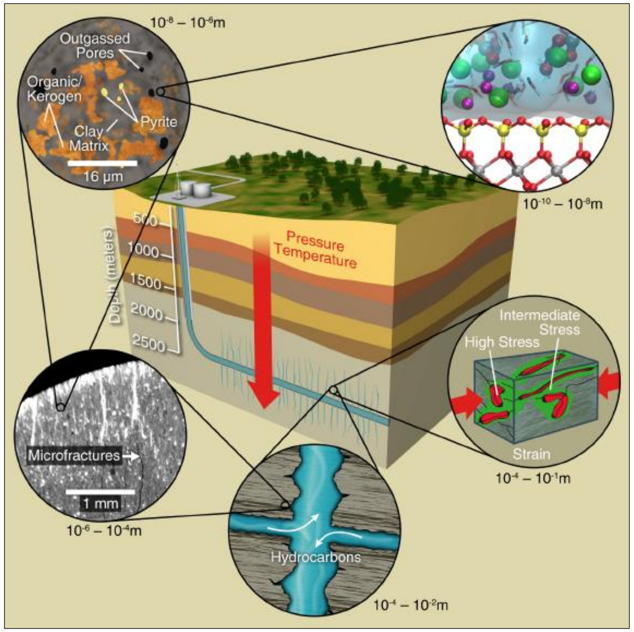
OUTCOME: New theory, new forms of matter, and novel characterization techniques that achieve unprecedented levels of optical efficiency, enabling photonic thermodynamic cycles.

U.S. DEPARTMENT OF ENERGY | Office of Science
PHOTONICS AT THERMODYNAMIC LIMITS
Stanford University | Berkeley University of California | Harvard University | Caltech | Illinois

Center for Mechanistic Control of Water-Hydrocarbon-Rock Interactions in Unconventional and Tight Oil Formations (CMC-UF)

Anthony R. Kovscek (Stanford University); Class: 2018-2022

MISSION: To seek fundamental mechanistic understanding to achieve control over the various non-equilibrium chemical and physical processes occurring in shale that increases hydrocarbon production while decreasing the amount of produced water, contaminants, and the number of wells drilled.



https://cmc-uf.stanford.edu/

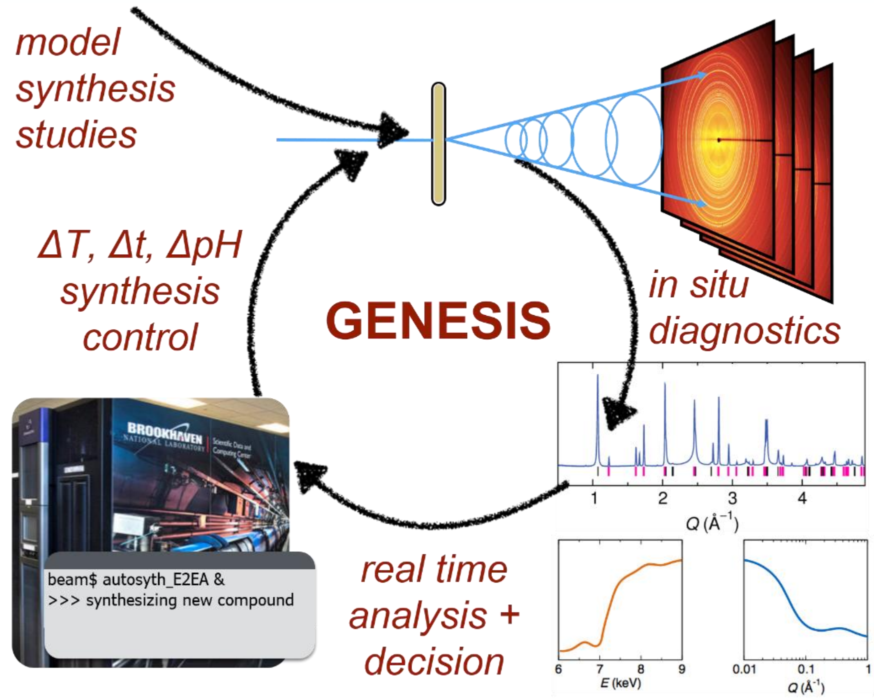
RESEARCH PLAN

Conduct a bottom-up, multiscale, multiphysics, multiphase, and multidisciplinary investigation of transport processes in nanoporous shales incorporating reactions with aqueous and nonaqueous fracture fluids and the mechanics of geomaterials.

A Next Generation Synthesis Center (GENESIS)

John Parise (Stony Brook University); Class: 2018-2022

MISSION: To develop a new paradigm for synthesis that accelerates the discovery of materials, by understanding how key structural and chemical transformations during synthesis are governed by the synthesis variables.



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

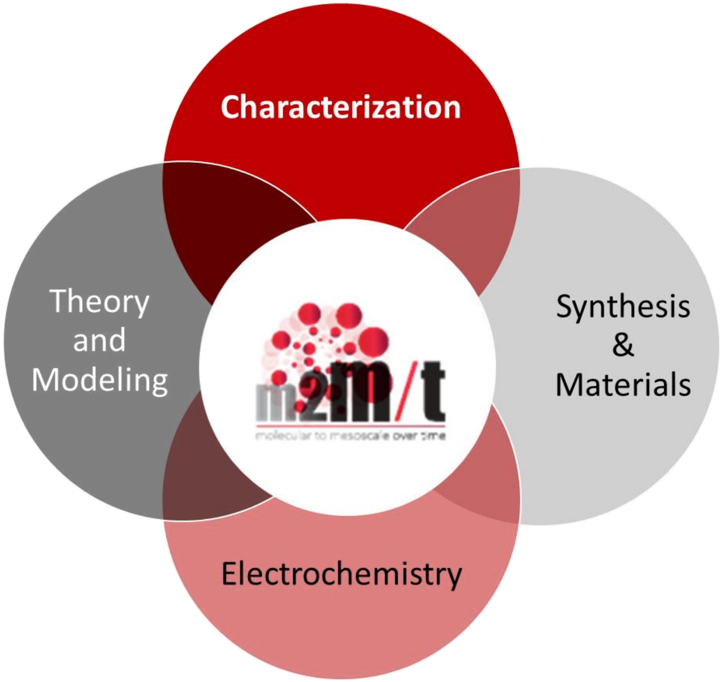
RESEARCH PLAN

GENESIS will accelerate the mapping of reaction space by integrating advanced in situ diagnostics and data science tools to interrogate, predict, and control reaction pathways. This will enable guided navigation of the pathways leading to new functional material targets.

Center for Mesoscale Transport Properties(m2m/t)

Esther S. Takeuchi (Stony Brook University); Class: 2014-2022

MISSION: To build the scientific knowledge base necessary to enable future creation of scalable electro-chemical energy storage systems with high energy, high power, and long life.



http://stonybrook.edu/m2m

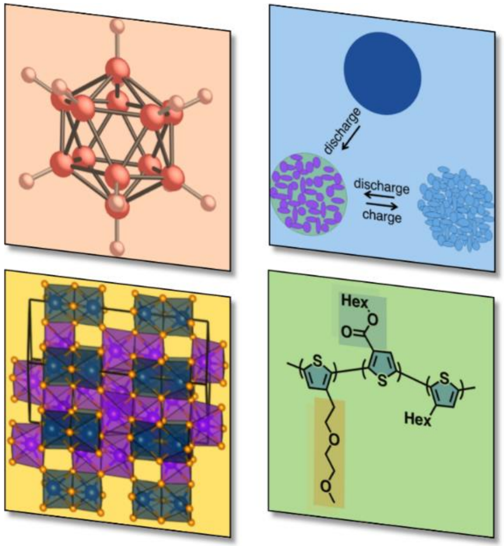
RESEARCH PLAN

The mission will be accomplished through the following initiatives: synthesize and investigate multifunctional materials with facile transport, understand and control dynamic interfaces, and rationally design electrode architectures.

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

Sarah Tolbert (University of California, Los Angeles); Class: 2018-2022

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



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

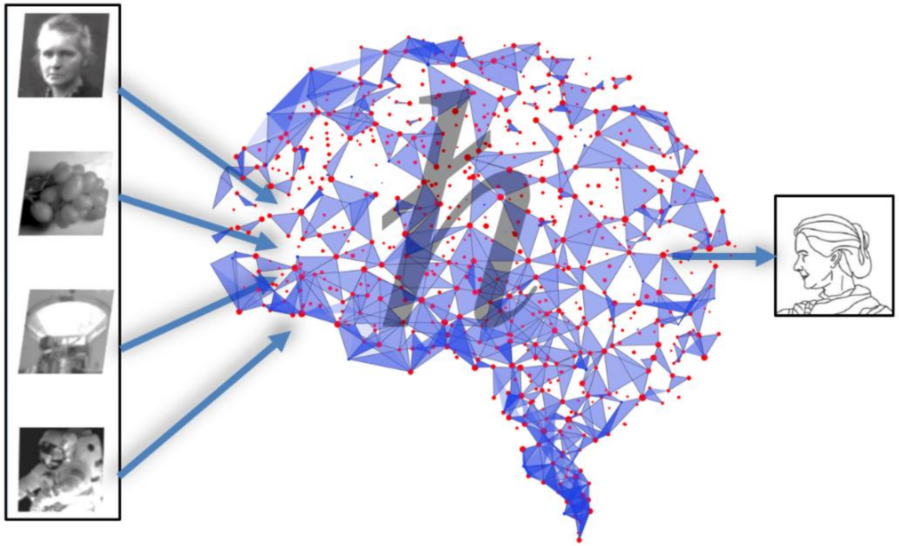
RESEARCH PLAN

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 achieve this goal, the team 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.

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

Ivan K. Schuller (University of California, San Diego); Class: 2018-2022

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").



A neuromorphic computer readily distills the image of a famous scientist from multiple inputs.

https://efrc.ucsd.edu

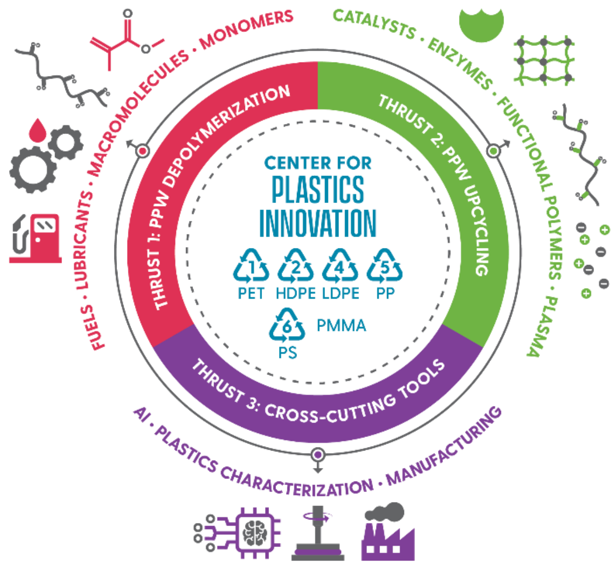
RESEARCH PLAN

Q-MEEN-C will breakaway from the conventional Turing-von Neumann paradigm by developing quantum materials for new types of bio-inspired ("neuromorphic") devices. Their exotic properties will be harnessed to develop completely novel functionalities: artificial synapses, neurons, axons, and dendrites that can be used to construct machines with artificial intelligence.

Center for Plastics Innovation (CPI)

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

MISSION: To develop catalytic and functionalization approaches and fundamental tools applicable to the upcycling of polymer plastics waste, with a strategic focus on enabling mixed-stream transformations from varied material form factors.



https://cpi.udel.edu

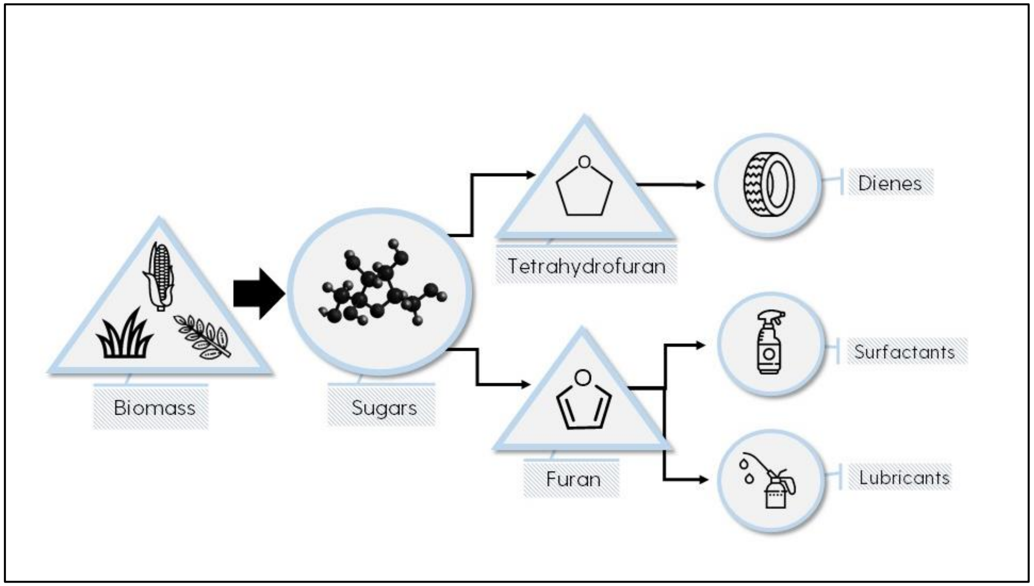
RESEARCH PLAN

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. CPI's vision is that these fundamental breakthroughs will enable efficient and selective processes to overcome the environmental impacts of increasing plastics waste.

Catalysis Center for Energy Innovation (CCEI)

Dionisios G. Vlachos (University of Delaware); Class: 2009-2022

MISSION: To advance the catalysis science of complex systems with a focus on thermocatalytic transformation of lignocellulosic (non-food-based) biomass into chemicals and transportation fuels.



https://www.ccei.udel.edu/

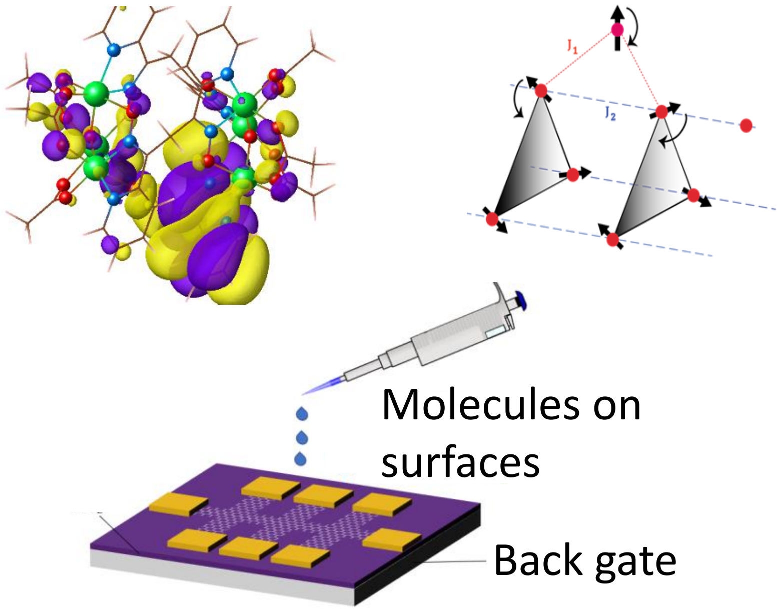
RESEARCH PLAN

Development of multifunctional, multiscale materials for enhanced energy efficiency by integrating kinetics and catalysis, synthesis of new and model materials with tailored architectures, development of imaging and operando spectroscopic techniques for characterizations, and multiscale computations.

Molecular Magnetic Quantum Materials (M^2QM)

Hai-Ping Cheng (University of Florida); Class: 2018-2022

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.



www.efrc.ufl.edu

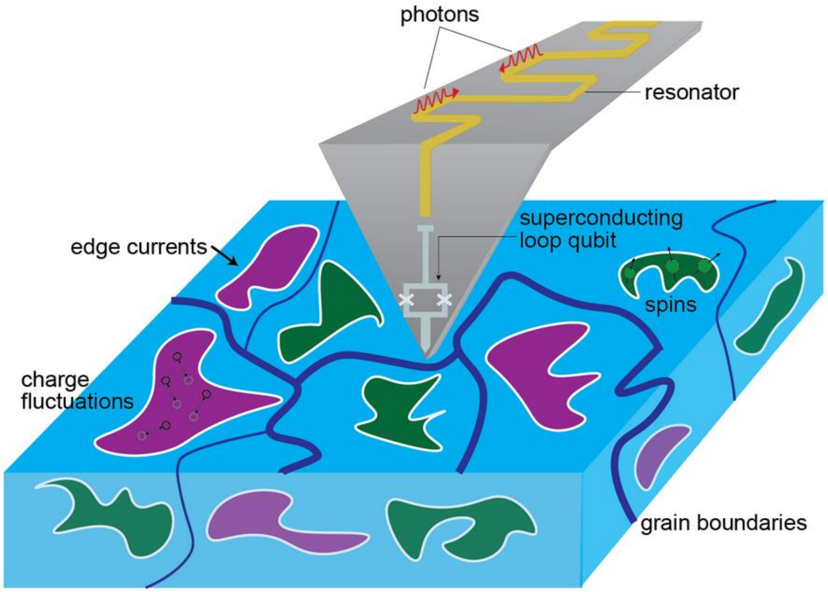
RESEARCH PLAN

Synthesize and characterize (experimentally and computationally) linked molecular magnets with various coupling strength, and study their resulting quantum properties and coupling to surfaces and junction interfaces. Study magneto-electric couplings and exotic spin phenomena in molecular solids.

Quantum Sensing and Quantum Materials (QSQM)

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

MISSION: To develop three new quantum sensing techniques—scanning qubit microscopy, two-electron Einstein-Podolsky-Rosen (EPR) spectroscopy, and nonlinear x-ray optics—and use them to study local and nonlocal quantum observables in quantum materials.



(Website URL TBA)

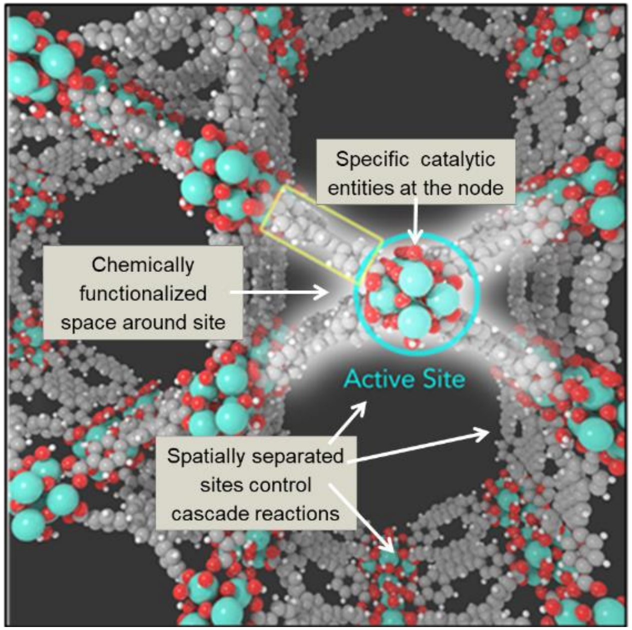
RESEARCH PLAN

QSQM will construct three new instruments, a scanning qubit microscope, a two-electron EPR spectrometer, and an x-ray four wave mixing setup. QSQM will use them to study the origin of exotic superconductivity, the signatures of topological order, and the nature of strange metal behavior in a wide variety of quantum materials.

Inorganometallic Catalyst Design Center (ICDC)

Laura Gagliardi (University of Minnesota); Class: 2014-2022

MISSION: To discover new classes of energy-science relevant catalytic materials, especially through the exploitation of computational modeling and artificial intelligence to identify underlying structure-function relationships that are critical to advancing further, predictive catalyst discovery.



http://icdc.umn.edu

RESEARCH PLAN

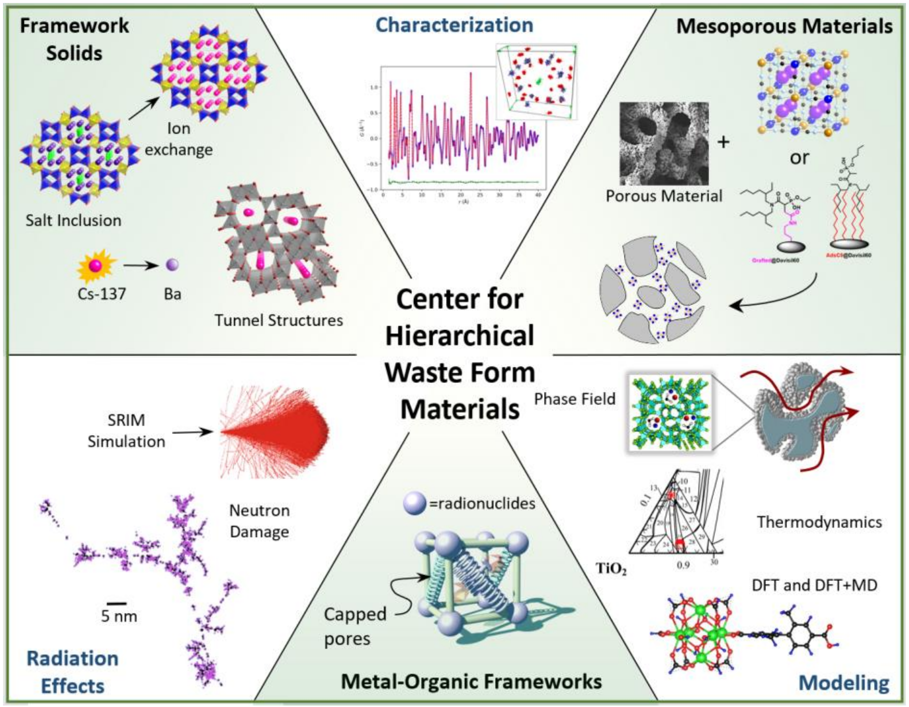
ICDC will advance computational and synthetic methods to create electronically and structurally well defined catalysts in mesoscale, hierarchically structured and uniform environments. Using rigorous theoretical and experimental techniques, ICDC will discover and rationalize structure/function relationships for atomically precise active sites and their surroundings.

U.S. DEPARTMENT OF ENERGY | Office of Science | ICDC INORGANOMETALLIC CATALYST DESIGN CENTER | THE UNIVERSITY OF CHICAGO | Northwestern University | MIT | NuMat Technologies | UC DAVIS | University of Minnesota | CLEMSON UNIVERSITY | Argonne National Laboratory | Pacific Northwest National Laboratory | Stony Brook University

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.



https://CHWM.sc.edu

RESEARCH PLAN

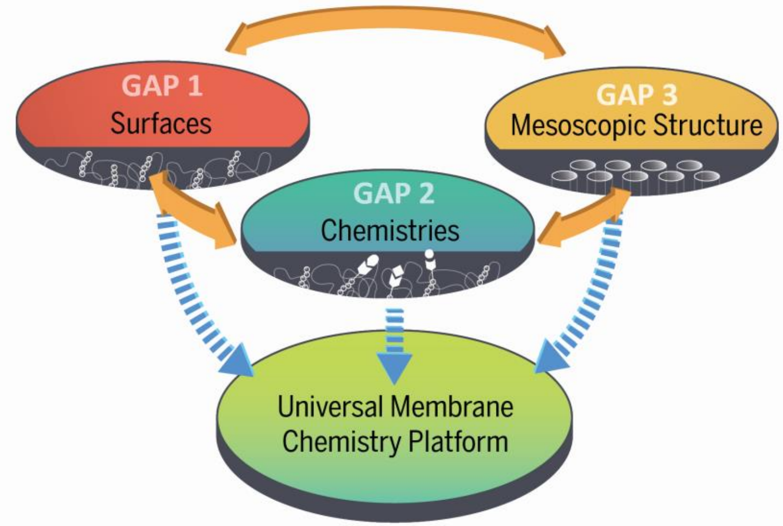
The CHWM aims to develop the basic science from which new nuclear waste forms can emerge. The Center will efficiently integrate experiment and modeling to develop chemistry and structure motifs that can lead to materials that effectively immobilize nuclear waste in persistent architectures.

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

Benny D. Freeman (The University of Texas at Austin); Class: 2018-2022

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

Integrating Framework



www.mwet.utexas.edu

RESEARCH PLAN

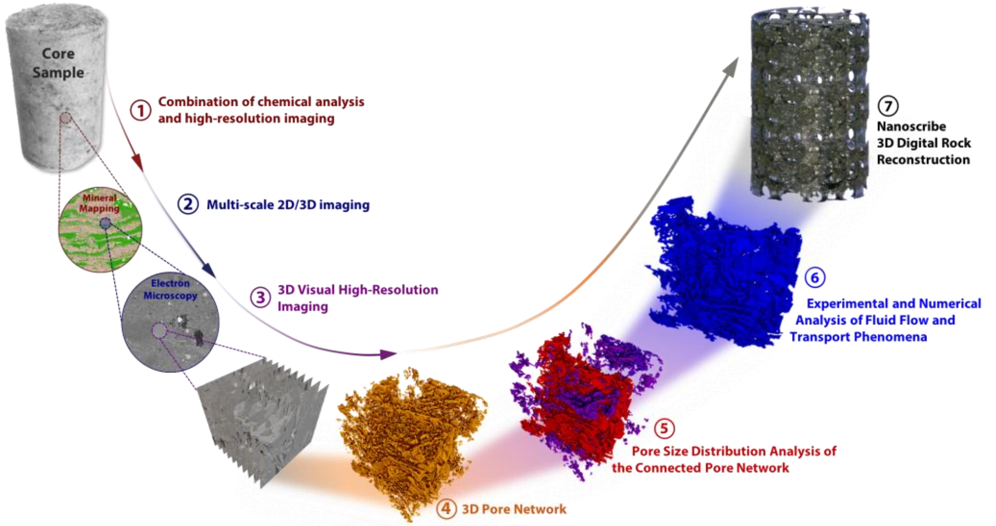
M-WET will integrate polymer synthesis, characterization and modeling to fill basic science gaps in the understanding of fluids and materials to design novel surfaces, highly selective solute/fluid interactions, mesoscopic structures, and membranes for energy applications.

U.S. DEPARTMENT OF ENERGY | Office of Science
M W E T CENTER FOR MATERIALS FOR WATER AND ENERGY SYSTEMS
TEXAS The University of Texas at Austin
UCSB
BERKELEY LAB

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

Darryl P. Butt (University of Utah); Class: 2018-2022

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.



www.EFRCMUSE.utah.edu

RESEARCH PLAN

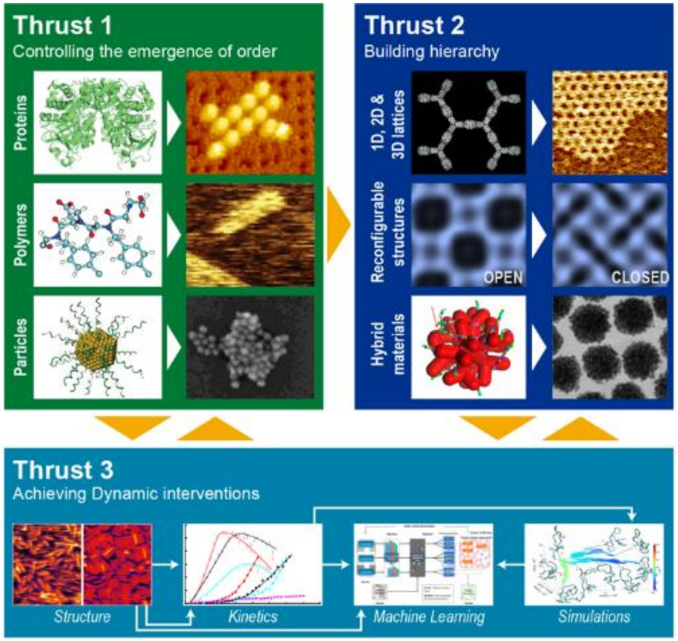
Synthesized geo-inspired materials will be used to probe the transport and interactions of multi-phase fluids over many length scales, including at the nanometer scale. Dynamic in-operando determination of material and fluid properties will be performed, and these measurements will be used for the development of experimentally-validated, atomistically-informed modeling tools and frameworks.

U.S. DEPARTMENT OF ENERGY | Office of Science | MUSE | Idaho National Laboratory

Center for the Science of Synthesis Across Scales (CSSAS)

François Baneyx (University of Washington); Class: 2018-2022

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



https://www.cssas-efrc.com

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.

GRAND CHALLENGES INDEX

TRANSFORMATIVE OPPORTUNITIES INDEX

BES REPORTS INDEX

TOPICAL INDEX

EXPERIMENTAL AND THEORETICAL METHODS INDEX