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**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.

**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.

[https://cats.ameslab.gov](https://cats.ameslab.gov)
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.

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.

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

**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.

[https://www.anl.gov/amews](https://www.anl.gov/amews)
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.

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

**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.

[https://www.bnl.gov/moltensalts/](https://www.bnl.gov/moltensalts/)
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.

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.

https://engineering.case.edu/EFRC BEES
MISSION: To discover, characterize, and deploy new forms of quantum matter controllable by gating, magnetic proximity and nanomechanical manipulation.

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.

https://quantum-materials.columbia.edu
**MISSION:** To achieve a detailed understanding of the nature, structure, and dynamics of electrocatalysis in alkaline media.

**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.
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.

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.

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

**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.

[https://efrc.gatech.edu](https://efrc.gatech.edu)
MISSION: To establish design principles for highly selective catalytic transformations driven by dilute alloys.

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.

https://efrc.harvard.edu/
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.

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.

https://teti.inl.gov/
MISSION: To realize, understand, and control revolutionary quantum materials and structures where quantum effects such as entanglement and coherence find collective macroscopic manifestations.

RESEARCH PLAN

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

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.
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.

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.

https://future.lanl.gov/
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.

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.

https://cent.mit.edu/
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.

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.

https://www.choise-efrc.org/
**MISSION:** To develop the next frontier in soft materials relevant to energy challenges by designing structures that emulate functions we see in biological systems.

**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.

[https://cbes.northwestern.edu](https://cbes.northwestern.edu)
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.

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.

https://cmqt.org
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.

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.
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.

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.

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

**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.

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

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.

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.

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.
MISSION: To exploit the 3\textsuperscript{rd} 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.

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

**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.

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

**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.

[https://ptl.stanford.edu](https://ptl.stanford.edu)
**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.

**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.

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

**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.

[https://www.stonybrook.edu/genesis/](https://www.stonybrook.edu/genesis/)

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A Next Generation Synthesis Center (GENESIS)
John Parise (Stony Brook University); Class: 2018-2022
MISSION: To build the scientific knowledge base necessary to enable future creation of scalable electrochemical energy storage systems with high energy, high power, and long life.

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.
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

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.
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.
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.

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.

https://cpi.udel.edu
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.

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.

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

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.

Molecules on surfaces
Back gate

www.efrc.ufl.edu
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.

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.
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.

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.

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

RESEARCH PLAN
The 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.

https://CHWM.sc.edu
**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.

**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.
**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.

**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.

www.EFRCMUSE.utah.edu
**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.

**RESEARCH PLAN**

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

https://www.cssas-efrc.com
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