Physical Sciences

Center for Nanophase Materials Sciences

Provides national and international user community access to expertise and equipment for a broad range of nanoscience research, including nanomaterials synthesis, nanofabrication, imaging/microscopy/characterization, and theory/modeling/simulation

Nanomaterials Characterization

Develops and applies state-of-the-art imaging and spectroscopy methods to understand the structure and function of complex materials in support of the CNMS user program and theme science.

1. *Functional Scanning Probe Microscopy* — Understands complex interplay between fields and materials at the nanoscale using novel scanning probe imaging and spectroscopy techniques via combined development of state-of-the-art instrumentation, controls, and advanced analysis methods.
2. *Microanalysis of Materials* — Understands materials structure, chemistry, and function by application of analytical and in situ STEM-based methods including cryo-EM.
3. Multimodal Imaging — Interrogates materials behavior by combining chemical imaging methods across multiple length and time scales.
4. *Scanning Transmission Electron Microscopy (STEM)* — Develops and advances new STEM-Scanning Electron Energy Loss Spectroscopy (EELS) techniques and push the spatial, temporal, and energy resolution limits for imaging and spectroscopy.
5. *Ultra-High Vacuum (UHV)-Scanning Tunneling Microscopy (STM)* — Develops novel capabilities to enable unprecedented insight into electronic, magnetic, and transport properties in low-dimensional systems and understand fundamental behavior of quantum systems.

Nanomaterials Synthesis

Develops innovative methods to precisely synthesize, process, and characterize functional macromolecules, nanomaterials, and nanostructures to understand structure, property, and function in support of the user program and theme science.

1. *Functional Hybrid Nanomaterials* — Conducts controlled synthesis of functional nanostructures and thin films by CVD and PLD using real-time diagnostics, e.g., 2D layered materials, hybrid organic/inorganic films, carbon nanostructures, oxide thin films, and heterostructures.
2. *Macromolecular Nanomaterials* — Performs precise synthesis of functional polymers with special emphasis on selective deuteration, small molecule synthesis, and ionic polymerization, as well as macromolecular characterization.
3. *Nanofabrication Research Laboratory* — Develops methods to fabricate nanostructures using best-in-class lithographic, etching, thin-film deposition, and characterization tools.

Theory and Computation

Advance computational capabilities and develop predictive models/simulations to further our understanding of the physical, structural, and chemical nature of nanomaterials and reactions, and integrate AI/ML methods into experimental platforms to enhance data analytics, efficiency, and the drive toward automation.

1. *Data Nanoanalytics* — Integrates edge computing and AI/ML methods into instrumentation and materials synthesis platforms to accelerate the pace of discovery.
2. *Nanomaterials Theory Institute* — Provides and advances capabilities for theory and high-performance simulation to enable fundamental understanding of physical and chemical properties of nanoscale materials and soft matter.

Chemical Sciences

Performs discovery and use inspired research to understand, predict, and control the physical processes and chemical transformations, relevant to energy technologies, over a broad range of length and time scales

Chemical Transformations

Performs research to understand and control chemical transformations at interfaces through design and synthesis of new materials and studying the reactivity of natural and synthetic systems.

1. *Energy Storage* — Understand and control the fundamental properties and processing of electrochemically and catalytically active materials to optimize charge flow and functionality.
2. *Geochemistry and Interfacial Sciences* — Understand and predict geochemical reactivity and mechanisms occurring at mineral-water interfaces and within porous media.
3. *Surface Chemistry and Catalysis* — Understand surface chemistry and catalytic reaction pathways to design and synthesize new, highly selective metal, metal oxide, and supported metal catalysts.

Nuclear Analytical Chemistry

Develops, advances, and applies analytical methodologies for elemental and isotopic characterizations in environmental and nuclear matrices to support ORNL and DOE mission

1. *Chemical and Isotopic Mass Spectrometry* — Develops and applies ultra-trace analytical measurements to address national and international nuclear safeguards, security, nonproliferation, verification, forensics missions, and stable and radioisotope production efforts.
2. *Radioactive Materials Analytical Laboratory* — Advances and applies radiochemical and mass spectrometry protocols for detailed characterizations of environmental and nuclear matrices within the nuclear fuels cycle and for production of anthropogenic and medical isotopes.

3. *Transuranium Analytical Laboratory* — Advances and applies radiochemical and mass spectrometry protocols for detailed characterizations of high-level nuclear matrices within the nuclear fuels cycle and for production of heavy isotopes in support of ORNL mission.

Separations and Polymer Chemistry

Designs and synthesizes new functional materials through understanding chemical and physical processes over a wide variety of length and timescales

1. *Carbon and Composites* — Designs and develops new feedstocks and processes for carbon, polymer, and fiber reinforced composite material systems for a variety of applications including structural and multi-functional materials and materials for extreme environments.
2. *Chemical Separations* — Develops highly selective receptors, membranes, and processes for the recognition and separation of ions and solid phases from aqueous solutions through fundamental understanding molecular interactions.
3. *Nanomaterials Chemistry* — Design and synthesize functional nanostructured materials and task specific ionic liquids to gain a fundamental understanding to advance chemical separations, catalysis, and energy storage.
4. *Soft Matter* — Develops fundamental understanding of the physical and chemical phenomena in soft matter, including synthetic and bio-polymers, polymer nanocomposites, and ionic liquids, and applies this knowledge to design of novel functional and adaptive materials.

Materials Science and Technology

Conducts fundamental and applied materials research for basic energy sciences programs and a variety of energy technologies, including energy efficiency, renewable energy, transportation, conservation, fossil energy, fusion energy, nuclear power, and space exploration

Foundational Materials Science

Understands, controls, and characterizes heterogeneities across length scales and their impact on structure and properties

1. *Correlated Electron Materials* — Performs research to understand and control bulk crystalline systems whose behavior derives from strong correlation effects of electrons and the resulting in superconducting, semi-conducting, magnetic, and thermoelectric properties.
2. *Neutron and X-ray Scattering and Thermophysics* — Develops and applies unique diffraction and thermophysical property measurement methods to characterize phase stability, residual stress, texture, thermal transport and thermal imaging of complex materials.
3. *Quantum Heterostructures* — Designs and synthesizes new functional oxides, topological quantum materials, artificial crystals, epitaxial thin films, and heterostructures by pulsed-laser deposition and molecular beam epitaxy.

Materials Structure and Processing Science

Understands, develops and applies advanced processing techniques to obtain desired materials structures and properties across length scales

1. *Alloy Behavior and Design* — Develops fundamental understanding of how to design and synthesize structural and functional alloys (e.g. HEA) for extreme environments based on advanced microstructural characterization, and modelling and design techniques.
2. *Materials for Advanced Manufacturing* — Designs, fabricates and characterizes the next generation of materials for use in advanced manufacturing.
3. *Materials Joining* — Advances materials joining science through development of new joining technologies by understanding weld microstructure evolution, properties and performance.
4. *Materials Processing* — Designs and develops next generation advanced processing techniques for development of hybrid and refractory materials for application in extreme environments by understanding processing pathways and thermodynamic/kinetics (e.g., CVD, CVI, densification).

Materials in Extremes

Understands and characterizes the effect of extreme environments on materials structure and properties to provide insights into mitigating these effects

1. *Advanced Nuclear Materials* — Understands the role of damage modes on the properties, structure and failure of structural materials and components for light water reactors, advanced fusion reactors, and DoD systems.
2. *Corrosion Science and Technology* — Develops solutions to environmental degradation through application of fundamental mechanistic understanding, advanced characterization techniques, and laboratory simulation of extreme environments.
3. *Mechanical Properties and Mechanics* — Understands the relations between processing, microstructure and mechanical properties of materials and how these change as a function of time, stress, temperature and environment through mechanical evaluation.
4. *Core Characterization Capabilities* — Provides custom fabrication of alloys, test samples for microscopy, and mechanical testing, physical properties measurement, and microstructural characterization of irradiated samples in the LAMDA.
5. *Radiation Effects and Microstructural Analysis* — Develops the fundamental knowledge to characterize the effects of radiation on material properties, to assist in determining the lifetime of irradiated components in reactors and develop strategies to mitigate the effects of high dose environments.

Materials Theory, Modeling & Simulation

Applies advanced computational and data analytic techniques to enable fundamental understanding and predictive control of new materials synthesis, fabrication and characterization across length scales.

1. *Materials Theory* — Advances the understanding of materials properties, especially strongly correlated materials, to design new materials with complex and emergent functionalities by application and development of theoretical and computational approaches.
2. *Microstructural Evolution* — Develops and applies advanced materials models to understand microstructural evolution during solidification and processing.

Physics

Builds on ORNL strengths to perform outstanding leadership research for the Nation in nuclear science, isotopes, and related areas. Our focus is in the areas of Fundamental Symmetries, Nuclear Structure Physics, Nuclear Astrophysics, Theoretical Physics, High Energy Physics and Heavy Ion Collisions and the associated Advanced Radiation Detector Development and Applied Data Science.

Fundamental Nuclear and Particle Physics

Unlocks the mysteries of the universe by studying the infinitely large and infinitely small

1. *Neutrino Research* —Leads the search for the rare neutrino-less double-beta decay process in ^{76}Ge, establishes leadership in fundamental neutrino physics (at the SNS and HFIR) and grows programs in high energy physics, nuclear non-proliferation and dark matter searches.
2. *Neutron Symmetries* — Probes the origin of the matter-antimatter asymmetry with neutron-based experiments at the SNS and develops a continuing program at the Second Target Station and/or HFIR.
3. *Relativistic Nuclear Physics* — Maps the quark - gluon structure and dynamics of strongly interacting matter including the proton and nuclei at the future Electron Ion Collider and the quark gluon plasma through heavy ion experiments at the Large Hadron Collider.

Nuclear Science and Advanced Technology

Delivers foundational knowledge in nuclear science and astrophysics through world-leading theoretical and experimental studies, as well as associated radiation detection technologies for next generation nuclear solutions needed by the nation and the world.

1. *Nuclear Structure and Astrophysics* — Delivers foundational knowledge of the understanding of the cosmic origin of nuclei and their properties, decays, and interactions, the physics of exploding stars and nuclei at the extreme limits of stability and mass, and informs real-world challenges in nuclear science; develops world-leading theoretical approaches by *ab initio* nuclear physics calculations and studies of nucleosynthesis and the astrophysical sites of this nucleosynthesis using high-performance computing.
2. *Advanced Radiation Detection, Imaging, Data Science, and Applications* — Research and development for understanding and exploiting combined signatures from radiation decay, radiography/tomography, system modeling and detection networks for use over a range of fundamental physics, next-generation advanced conceptual systems, and current real-world applications