



Center for Nanophase Materials Sciences

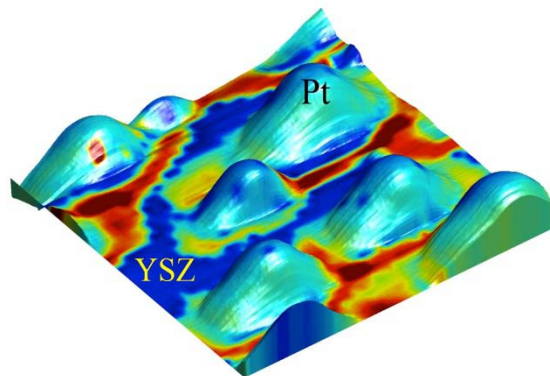
The Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory (ORNL) integrates nanoscale science with neutron science; synthesis science; and theory, modeling, and simulation. Operating as a national user facility, the CNMS supports a multidisciplinary environment for research to understand nanoscale materials and phenomena.

Scientific Themes

CNMS research focuses on understanding, designing, and controlling the dynamics, spatial chemistry, and energetics underlying functionality and properties of nanoscale materials, systems, and architectures.

Electronic and Ionic Functionality on the Nanoscale

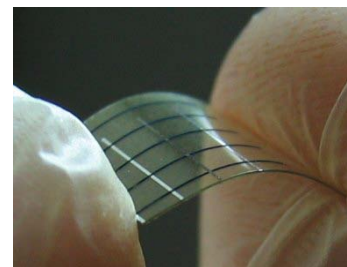
- Developing instrumentation and techniques to image and understand the functionality of nanoscale materials and interacting assemblies
- Research on optoelectronic, ferroelectric, ionic and electronic transport, and catalytic phenomena at the nanoscale
- Understand energy transfer at nanoscale interfaces



Activity of oxygen reduction at a surface of a fuel cell material is accelerated at the triple phase boundary between air, platinum particles, and ionic conductor, as mapped by Electrochemical Strain Microscopy.

Functional Polymer and Hybrid Architectures

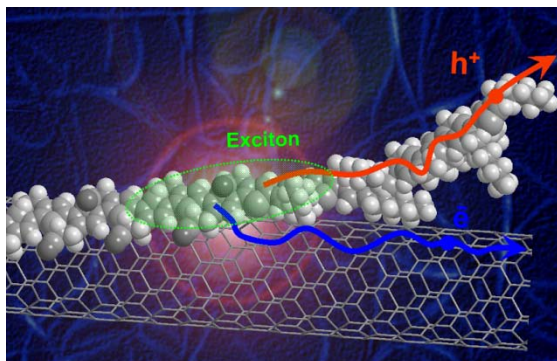
- Advancing our fundamental understanding of the links between polymer structure, property and function that are controlled by weak intermolecular interactions and interfacial phenomena
- Understanding the role of macromolecular topology in self-assembly
- Understanding how the optoelectronic properties of conjugated material architectures and hybrid systems are determined by their structure



A flexible plastic cross-point memory device based on a network of Cu-TCNQ nanowires

Collective Phenomena in Nanophases

- Builds on strong theoretical and experimental efforts focusing on understanding the emergence and ramifications of collective behavior
- Developing and applying multiscale methods to understand and predict how atomic structure, nanoscale confinement, and quantum mechanical effects impact electronic processes/properties within materials and across interfaces
- Understanding nature's 'rules of composition' to enable synthetic nanostructured systems with capabilities rivaling those of living systems



Synthesis and processing of hybrid systems including well-defined interfaces and architectures to test and model



Coupling ultrafast with ultrasmall

Research Capabilities

The CNMS is housed in a beautiful facility on the Chestnut Ridge Campus of ORNL, co-located with the Spallation Neutron Source. It is equipped with a wide range of specialized tools for synthesis, characterization, and fabrication of novel nanoscale materials and assemblies, including the integration of hard and soft materials. CNMS encompasses expertise and instrumentation for user research in a broad range of disciplines selected to address forefront research in nanoscience and nanotechnology.

- **Macromolecular Nanomaterials:** Synthesis and molecular level characterization of small molecule building blocks, polymers, and polymer-modified interfaces, including biologically inspired systems, deuterated molecules and polymers for neutron scattering studies.
- **Functional Hybrid Nanostructures:** Specialized laser and CVD synthesis of carbon nanomaterials, oxide heterostructures, nanoparticles, and organic nanowires with real-time diagnostics. Processing, electronic/optical measurements, and environmental testing of oxide electronics and organic optoelectronics over multiple length scales.
- **Chemical Functionality:** Template- and surfactant-mediated synthesis of functional, nanostructured oxides and carbons; catalysis characterization; non-ambient and dynamic x-ray characterization and elemental analysis; battery characterization; multi-wavelength Raman; electron microscopy including EELS, soft-matter TEM, cryo-TEM, energy-filtered imaging, SEM and STEM.
- **Imaging Functionality:** Scanning probe microscopy for imaging and dynamics in nanostructures including ionic and electronic transport, electromechanics, energetics, magnetic domains, chemical reactions, and electronic, structural and spin phases and transitions.
- **Nanomaterials Theory Institute:** Multiscale modeling, nanomaterials design, virtual synthesis and characterization using high performance computing capabilities.
- **Nanofabrication Research Laboratory:** Controlled synthesis and directed assembly of nanomaterials in a Class 1000 cleanroom environment; chemical and biological functionalization of nanoscale materials.

Many user projects take advantage of multiple capabilities in tackling research to understand complex nanoscale phenomena. In addition, CNMS has partnerships with other ORNL user programs enabling users to access these facilities. The Nanomaterials Theory Institute provides collaborative workspaces, visualization equipment, and high-speed connections to the ultrascale computing facilities of the National Center for Computational Sciences. The intense neutron beams from the Spallation Neutron Source and from the High Flux Isotope Reactor afford unique and expanding opportunities for fundamental studies of the structure and dynamics of nanomaterials. The CNMS also provides a gateway to sub-angstrom electron microscopy, atom probe, and other capabilities in the Shared Research Equipment user program.

User Program

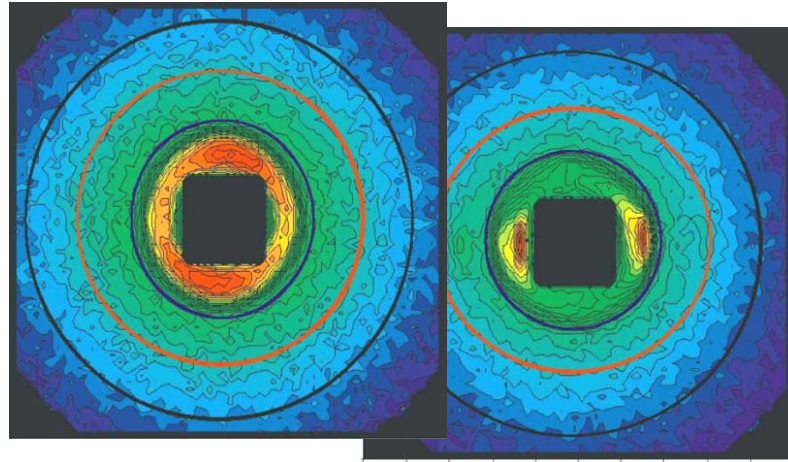
The CNMS user program provides access to equipment and technical expertise for nanoscale research that defines the state of the art. The program is open to users from academia, the private sector, and research institutes worldwide. Users join a vibrant research community that brings together ORNL research staff, technical support staff, students, postdoctoral fellows, and collaborating guest scientists. The program accommodates both short-term and long-term collaborative research partners. Access is obtained through a brief peer-reviewed proposal with no charge for users who intend to publish their results. Access is available on a cost-recovery basis for research that is not intended for publication. Prospective users are encouraged to consult CNMS staff to learn more about the Center's science and capabilities.

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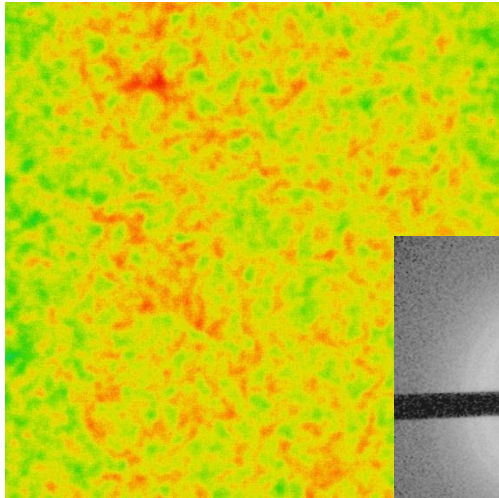
Macromolecular Nanomaterials

Scientific Focus

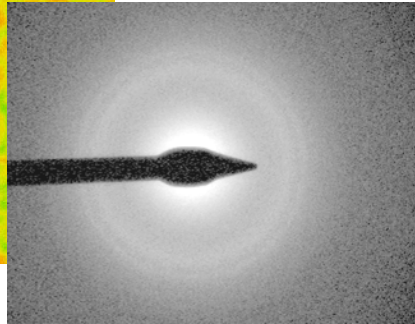
- Precisely-made and rigorously characterized polymers and block copolymers in support of users and CNMS science
- Deuterated monomers and polymers for neutron scattering
- Assembly-structure-property studies of conjugated polymers, synthetic bio-inspired polymers, and polymers having complex architectures
- Nanoscale characterization of ultra thin polymer films and interfaces



Small angle neutron scattering of deuterated block copolymers demonstrates how an applied electric field (left) alters structure and performance



Energy filtered TEM of P3HT and P3HT-b-PEO blend

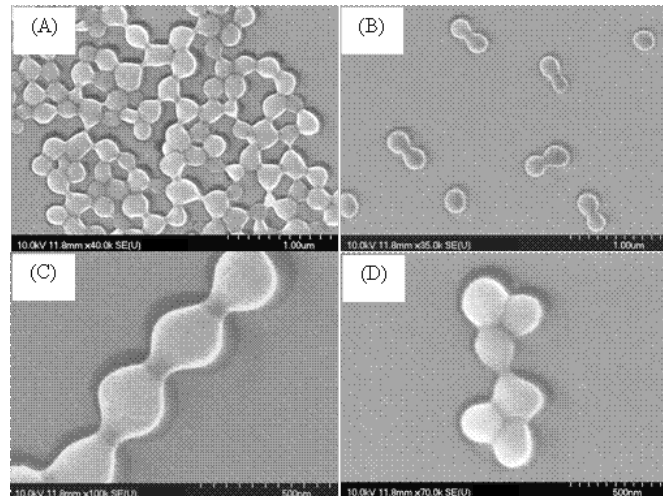


Electron diffraction of compatibilized blend

Complex micelles formed from fluorine-containing triblock copolymers

Capabilities

- Synthesis of well-defined, macromolecular nanomaterials by anionic, cationic, ROMP and controlled polymerizations, yielding linear, block, star, graft and dendrimeric architectures
- Synthesis of small molecule building blocks, deuterated monomers and polymers
- Characterization by spectroscopy, SEM and TEM microscopy, and chromatographic methods
- Thin film characterization and assembly



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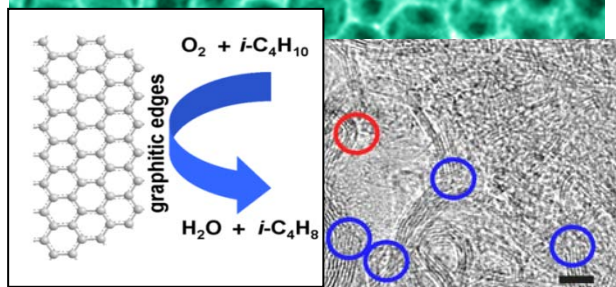
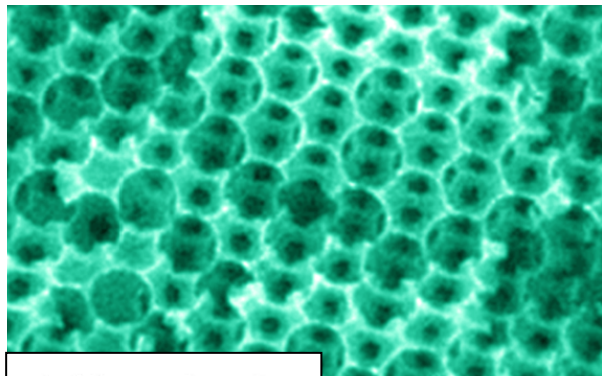
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Chemical Functionality

Scientific Focus

- Understand energy flow in nanoscale architectures and how macroscale functionality is determined - focusing on synthesis, structure, catalysis and energy storage.
- Develop novel methods to synthesize, process, and characterize inorganic/organic nanoscale building blocks with well defined structure, interfaces and architectures.
- Utilize coordinated chemical and physical probes to understand functional mechanisms of nanostructures.



Nanostructure Synthesis

- Template- and surfactant-mediated synthesis of mesoporous oxides and carbons for catalysts and functional supports
- Chemical, hydrothermal, solvothermal routes for nanoparticle synthesis
- Surface functionalization of oxides and carbon
- Atomic layer deposition (ALD) and surface sol-gel processing (SSG) for conformal functionalization of support surfaces
- Graphitization and carbonization



Characterization and Functional Testing

- Electron microscopy (TEM, SEM, STEM) including soft-matter, EELS, EDX, Cryo-TEM and energy-filtered imaging for soft-materials
 - Sub-angstrom resolution through SHaRE
- X-ray diffraction and small-angle scattering at temperature and pressure
 - Powder, thin-film
 - SAXS with grazing-incidence, humidity control, temperature, capillary, powders
- FY2013: Helium-ion microscopy; ultra high-resolution surface imaging.
- Operando, in situ characterization of reaction intermediates, surface species, and catalytic nanostructure: Raman, IR, DRIFTS, XRD
- Thermogravimetric and sorption measurements
- Cells, environments and collaborations for neutron scattering experiments
- Structural characterization of oxide and metal nanomaterials, surface and bulk structure
- Catalyst performance characterization including gas and condensed phase reactivity and selectivity
- High precision measurements of battery performance with controlled temperature
- Battery diagnoses through impedance measurements
 - Drybox for cell construction
- Elemental analysis with X-ray fluorescence and CHNS-O analyzer

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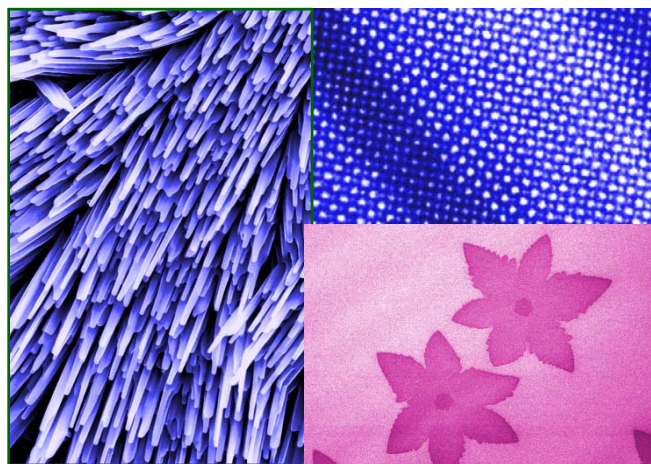
Functional Hybrid Nanostructures

Scientific Focus

- Develop novel methods to synthesize, process, and characterize primarily inorganic nanoscale building blocks with well defined structure, interfaces and architectures.
- Utilize coordinated multiscale probes to understand energy flow in hybrid architectures and how functionality emerges at multiple length scales.



Hybrid nanomaterials synthesis facility

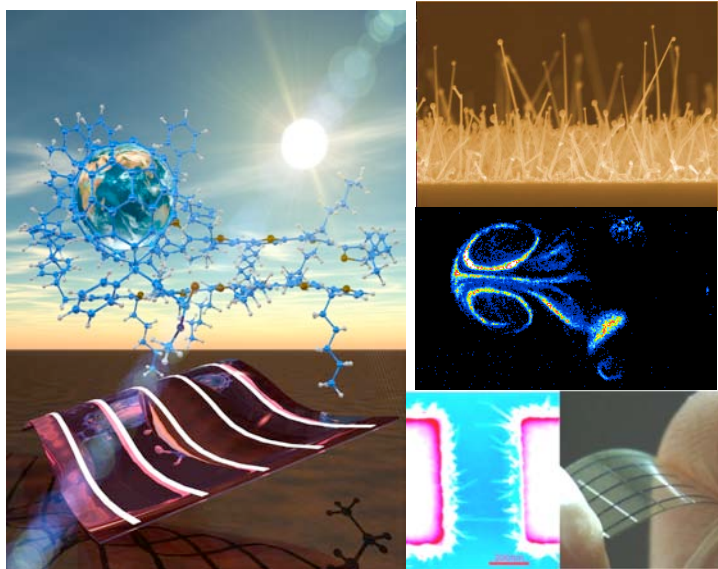


Characterization and Functional Testing

- Optoelectronic characterization and functional testing (UV-Vis-NIR, PL, Raman)
- Calibrated, OLED, PV, and OFET testing
- Tunable ultrafast laser spectroscopy (Raman, confocal micro-Raman, pump-probe)
- Electrical transport, semiconductor parameter analysis, four-point-probe, AC-impedance measurements.
- Ferroelectric and R-T measurements
- Thin film XRD at temperature and pressure

Nanostructure and Hybrid Material Synthesis and Processing

- Synthesis with time-resolved, in situ spectroscopic diagnostics and growth kinetics
- Carbon nanomaterials: SWNTs, SWNHs, MWNTs, VANTAs, graphene, by PVD and CVD
- Oxide thin films and heterostructures
- Crystalline organic nanowires by PVD
- Nanoparticles and nanowires by PLV, LA-CVD
- Sonospray patterning and large area deposition
- Inert-atmosphere glovebox processing for inorganic/organic hybrid electronics
- Nanoparticles by ultrafast laser vaporization and surface nanostructuring



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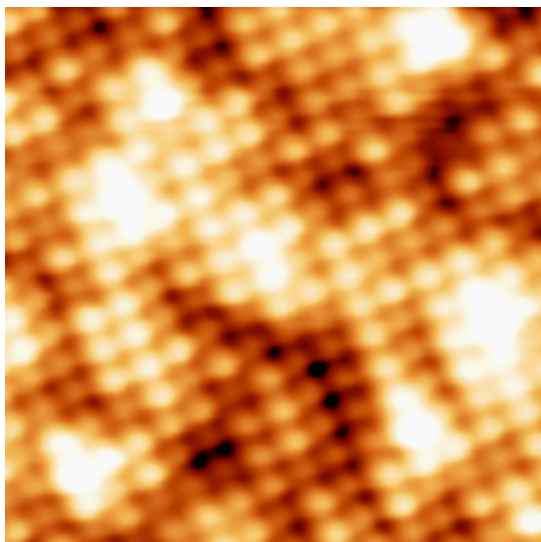
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Imaging Functionality

Scientific Focus

- Development of novel methods for probing and controlling materials functionality on the nanometer and atomic scales
- Dynamics of bias-induced and thermal phase transitions
- Mapping energy transformation pathways in ionic, magnetic, ferroelectric, molecular, and quantum systems
- Electronic and ionic transport in low-dimensional and energy systems
- Spin-resolved electron microscopy imaging
- High-resolution STM imaging and spectroscopy of molecular systems and correlated oxides

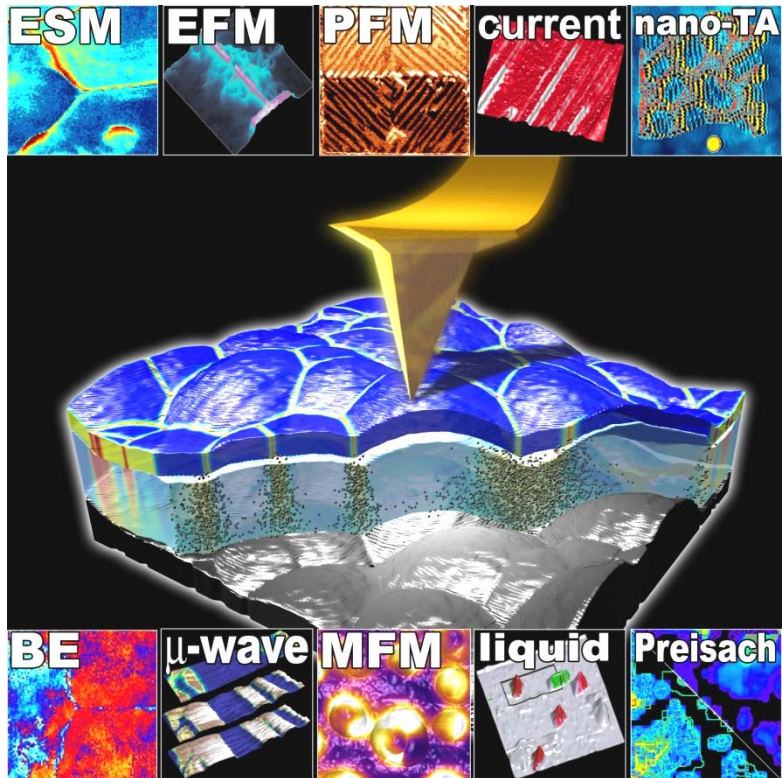


Atomic resolution of superconducting $\text{FeTe}_{0.55}\text{Se}$ at 4K

Unique Capabilities

- Suite of SPM tools with band excitation control
- In-situ oxide growth and SPM/surface science studies
- 4-probe STM system with MBE growth and SEM imaging for transport
- Low-T, high magnetic field and variable temperature STM and STS
- Variable temperature scanning electron microscopy with polarization analysis
- Electromechanical probes of ionic motion, ferroelectric, multiferroic, and energy materials
- Simultaneous piezoresponse force and conductance microscopy

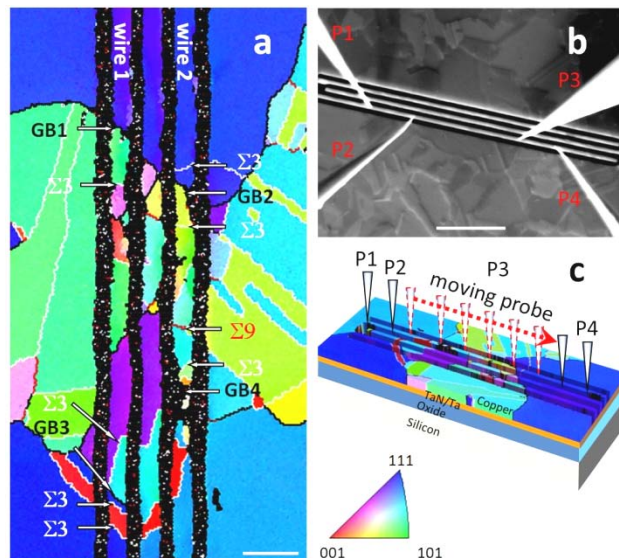
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Numerous properties can be measured with force based probes

User Support

- Access and support of advanced Scanning Probe Microscopy (SPM) modes
- Theory support for SPM data interpretation
- Access to expertise of ORNL SPM researchers
- Training and education in imaging techniques



4-Probe transport across individual Cu grain boundaries

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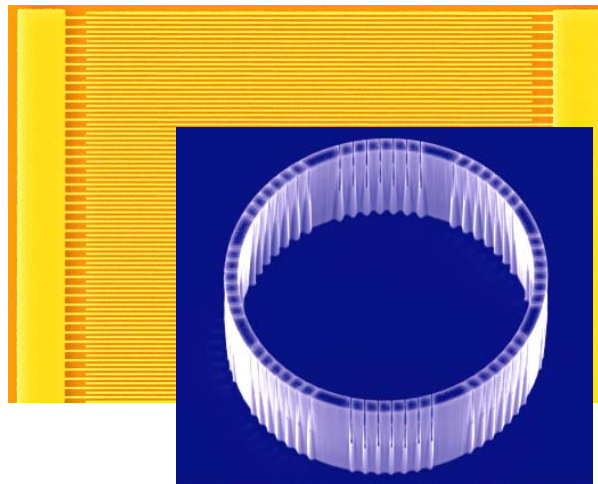
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Nanofabrication Research Laboratory

The NRL houses a full suite of micro- and nanofabrication capabilities supporting users in all CNMS Scientific Themes.

Multiscale Material Processing and Integration

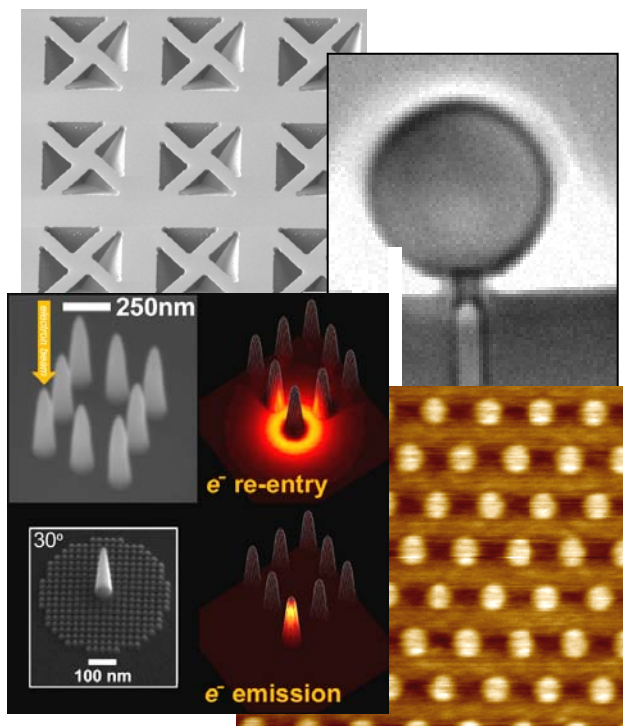
- **Facilities** – The NRL is equipped to manipulate and characterize a broad range of materials including dielectrics, metals, semiconductors, polymers and their composites
- **Nanolithography and Pattern Generation** – Advanced electron beam and ion beam lithography allow nanoscale patterns to be written directly on samples, while on-site mask writing capabilities facilitate rapid cycling from concept to pattern
- **Material Deposition and Etching** – High temperature furnaces, chemical vapor deposition, physical vapor deposition and atomic layer deposition techniques are complemented by reactive ion etching using both fluorine and chlorine etch chemistries



Scientific Focus

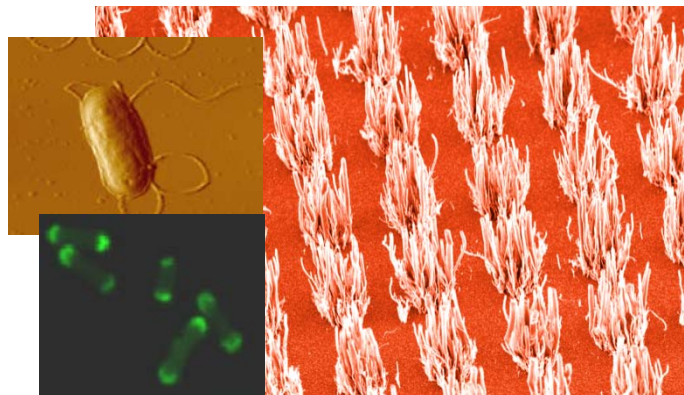
A diverse in-house research program continuously drives process and capability development within the NRL.

- **Molecular Transport in Nanoscale Systems:** Nano- and microfluidics are used to study chemical and biochemical reaction kinetics under dimensionally-restricted conditions
- **Nanomechanics:** Dynamics and transport properties of freestanding membranes and suspended structures are interrogated across multiple length scales
- **Soft Material Interfaces** – The influence of chemical and topographical templates on inorganic and biomimetic assembly processes is studied
- **Electron and Ion Beam Processing** – The FEI Nova 600 dual scanning electron microscope/focused ion beam system includes electron/ion beam lithography, energy dispersive spectroscopy and photon-assist capabilities with simulation capabilities that underpin the beam stimulated processing efforts



A Nano-enabled Approach to Biology

- **Imaging Biological Processes** - In partnership with affiliate laboratories, the NRL offers capabilities for imaging of biological materials using optical and scanning probe techniques
- **Interfacing with Soft Materials** – Interfaces developed using chemically patterned surfaces and microfluidic platforms leverage capabilities in nanolithography and material manipulation
- **Understanding emergent phenomena** - the above techniques are used to understand fluctuations in natural systems and emergence of complex behavior in biology



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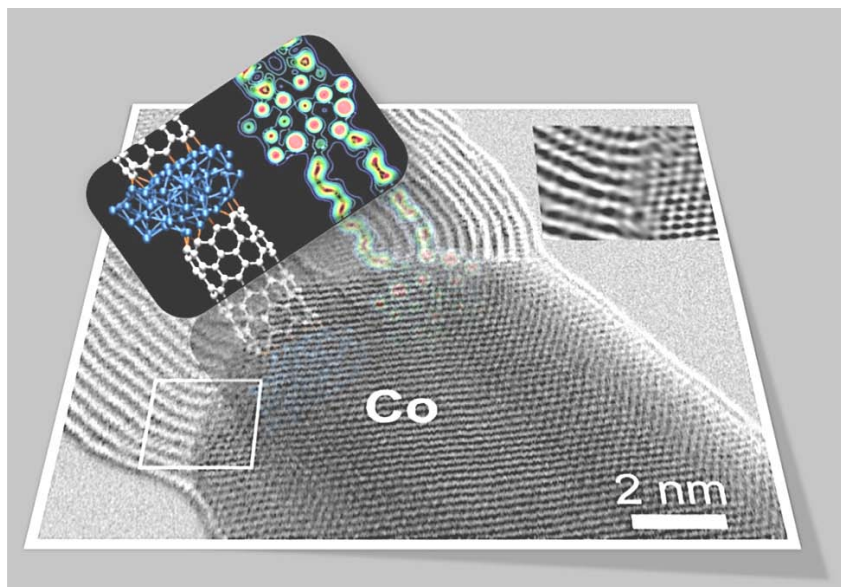
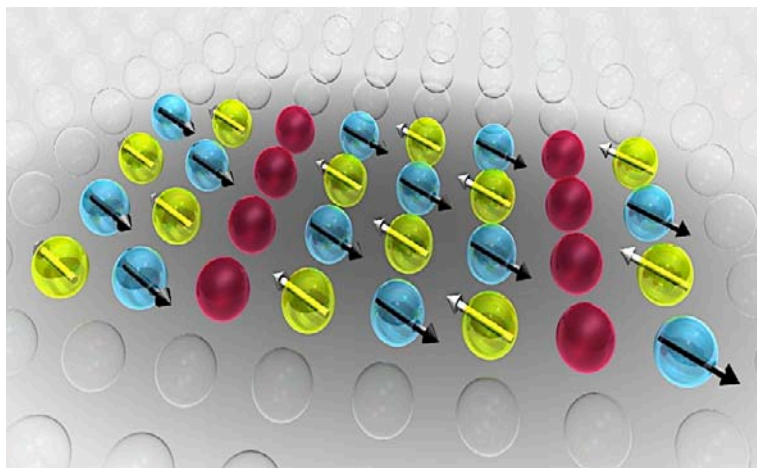
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Nanomaterials Theory Institute

Scientific Focus

- Development of methodologies for theoretical and computational nanoscience
- Promotion of community-based code development in areas relevant to theoretical and computational nanoscience
- Science focuses: Multiscale methods, electron transport, neutron scattering from nanostructures, nanostructures in hard, soft materials, electron correlation and magnetism, electron and spin transport, self-assembly and effects of confinement
- Computational nanoscience end-station for capacity and capability computing

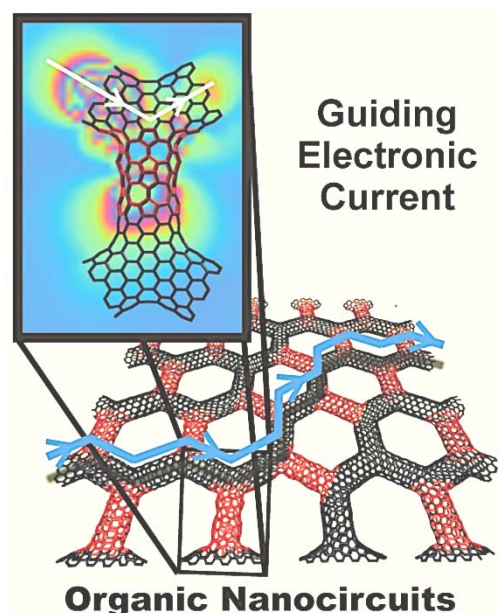


Facilities

- NTI Beowulf cluster (~21 TFlops)
- NTI Developmental Cluster (216 CPU cores and 12 Tesla/ FERMI cards)
- National Energy Research Supercomputing Center (NERSC) allocation – high-end capacity computing
- National Leadership Computing Facility (NLCF) allocation – capability computing
- 16-screen video wall and 16-quad-processor-node visualization cluster/data storage

User Support

- Theory/computational support for theory and experimental users/projects
- Access to NTI and facilitation toward use of ORNL computational resources
- Access to expertise of NTI and ORNL materials modeling researchers
- Formulation of theory/modeling support for experiment and/or instruments



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