Center for Nanophase Materials Sciences (CNMS)

Central Campus

SNS

Chestnut Ridge

CNMS
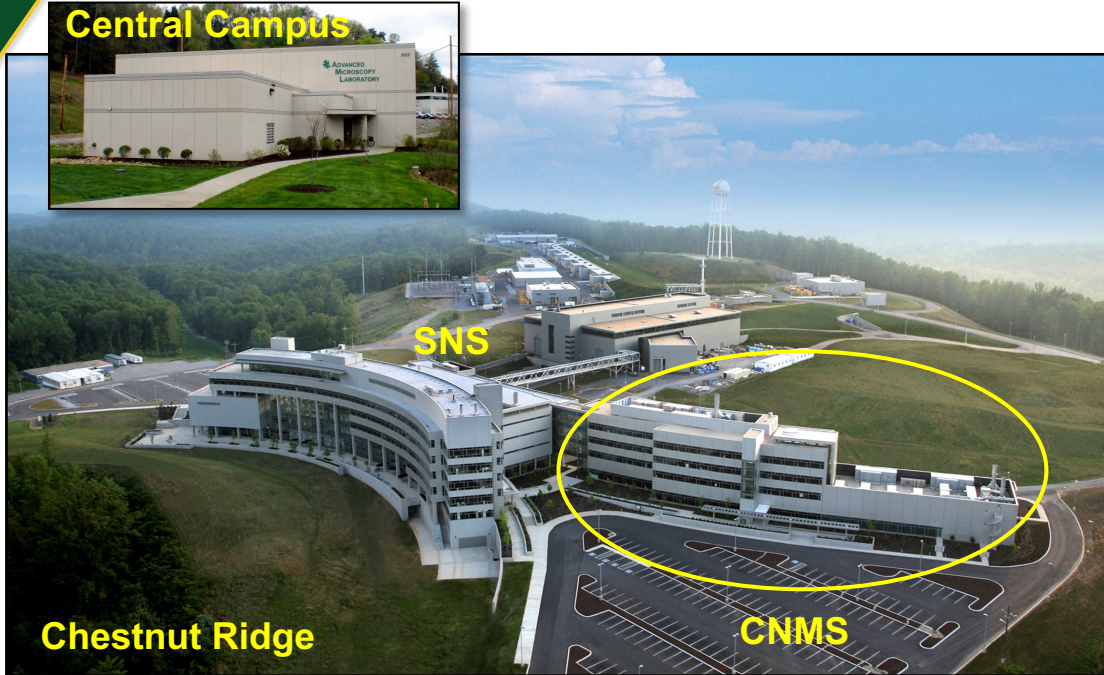
- Co-located with other BES user facilities
  - Spallation Neutron Source (SNS), High Flux Isotope Reactor (HFIR), and Oak Ridge Leadership Computing Facility (OLCF)
- 811 unique users in FY22
  - ~60% outside of TN (including international)
  - Recent investments in "remote operations"

- 520 Active User Proposals
- FY22 - 360 peer-reviewed publications
 - 55% in journals with IF > 7
  - 11 journal covers

U.S. DEPARTMENT OF ENERGY | Office of Science

Argonne NATIONAL LABORATORY | Center for Nanoscale Materials

Sandia National Laboratories

Los Alamos NATIONAL LABORATORY

MOLECULAR FOUNDRY

Brookhaven National Laboratory | Center for Functional Nanomaterials

OAK RIDGE National Laboratory | CENTER FOR NANOPHASE MATERIALS SCIENCES
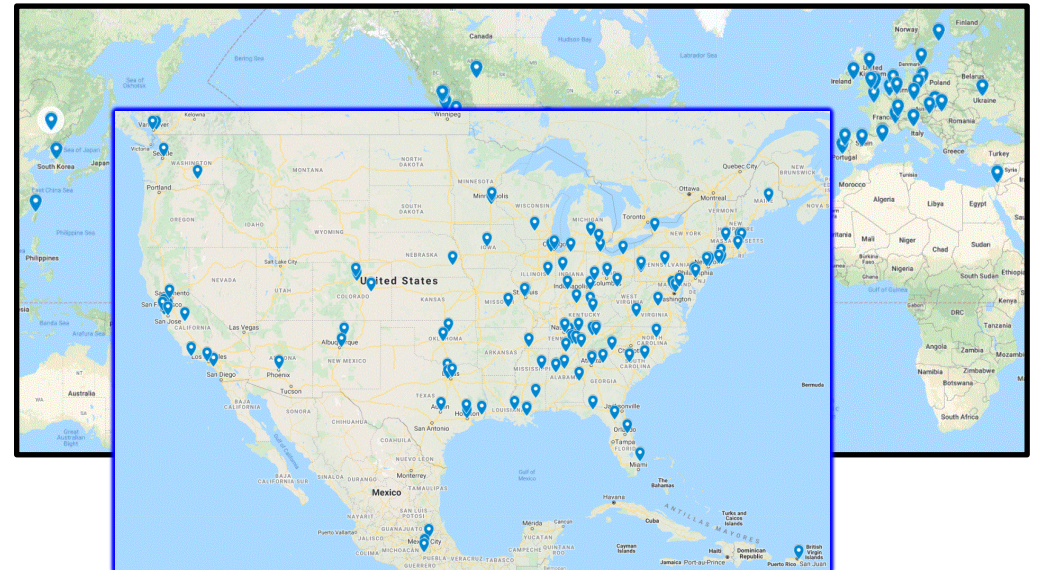
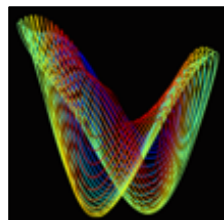# CNMS Scientific Impact Enables New User Science

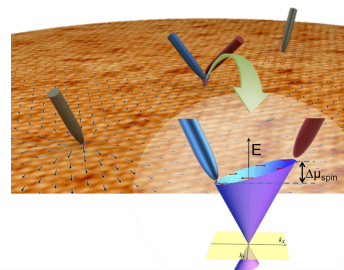## Imaging & Spectroscopy
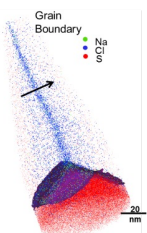
Atom probe tomography and application to non-conventional (non-metallic) nanomaterials
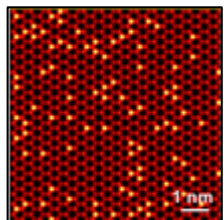
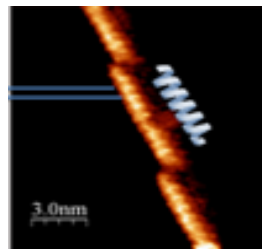Ultra-high energy resolution monochromated STEM-EELS; low voltage STEM; cryo-STEM

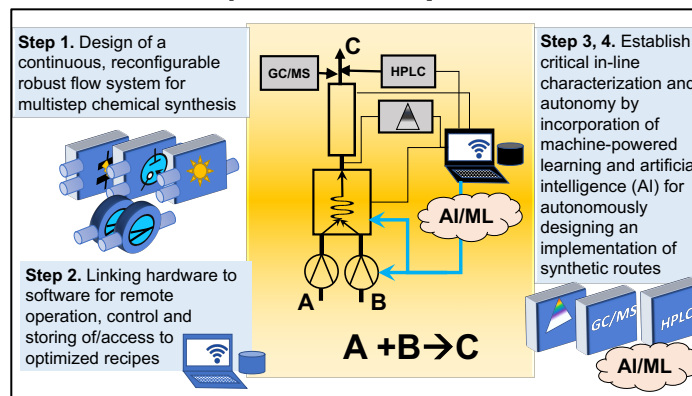Band-excitation and G-mode AFM, quantification of nanoscale electromechanical phenomena

Unique spin-polarized 4-probe STM, vector-field mK STM, Joule-Thomson STM
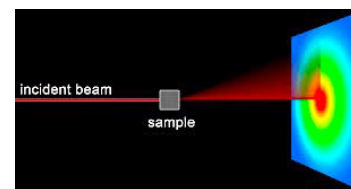
Soft Matter Science

- Precision synthesis of complex multiblock copolymer topologies
- Site-specific deuteration

- Autonomous continuous flow reactor synthesis (**AutoFlowS**)

Step 1. Design of a continuous, reconfigurable robust flow system for multistep chemical synthesis

Step 2. Linking hardware to software for remote operation, control and storing of/access to optimized recipes

Step 3, 4. Establish critical in-line characterization and autonomy by incorporation of machine-powered learning and artificial intelligence (AI) for autonomously designing an implementation of synthetic routes

A + B → C

- Significant effort to bridge simulations and data analysis with neutron scattering
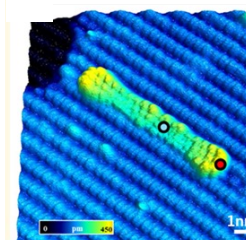

Autonomous Experimentation

- Autonomous synthesis
  - PLD, CVD, AutoFlowS
  - Nanofabrication and direct-write capabilities
  - EBID/IBID

- Autonomous microscopy and atomic manipulation & assembly
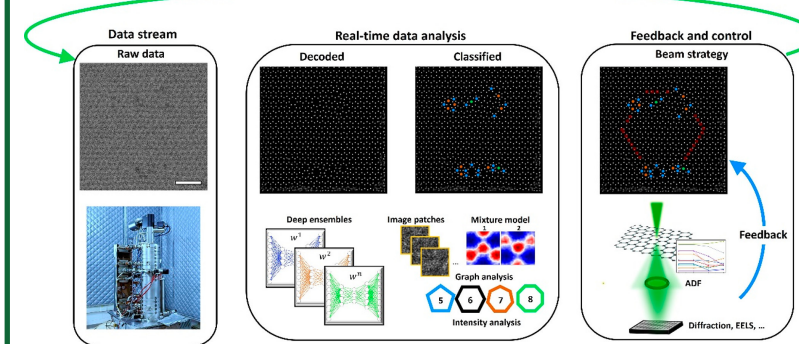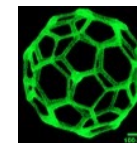
Roccapriore et al., *ACS Nano* **16** (2022)

Directed synthesis of atomically precise graphene nanoribbons for magnetic end states

Synergy with NSRCs and other BES User Facilities

- CNMS FY22 publications demonstrate synergy with multiple BES user facilities
- 129 shared users with SNS/HFIR
 - Soft Matter
  - Quantum materials

Pie chart: CNMS 60%, OLCF, NERSC, SNS/HFIR, Light Sources, Other NSRCs
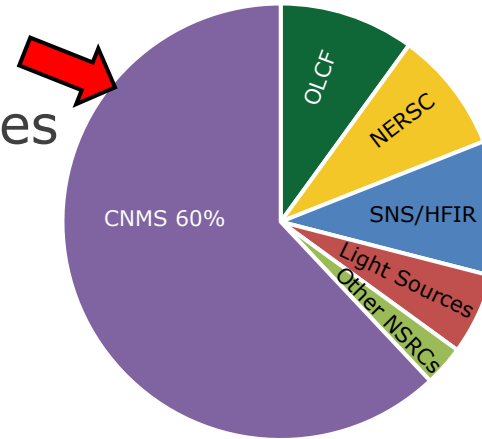
- Participation in SC Data Workshops/Reviews:
- Workshop Series: Advanced Research Directions on AI for Science and Security (AI4SS)
  - *Surrogates and AI for HPC & AI for Complex Systems*
  - *AI for Advanced Property Inference and Inverse Design*
  - *Foundational AI for Scientific Knowledge Discovery, Integration, and Synthesis*
- ESNet – BES Network Requirements Review

- Collaborations on other BES-SUFD programs:
  - Partner on 3 AI/ML at DOE Scientific User Facilities Projects
    - *4D Camera Distillery (LBNL)*
    - *Digital Twin for Spatiotemporally Resolved Experiments (ANL)*
    - *Collaborative ML Platform for Scientific Discovery (LBNL)*
  - NSRC Recapitalization Project (CFN)
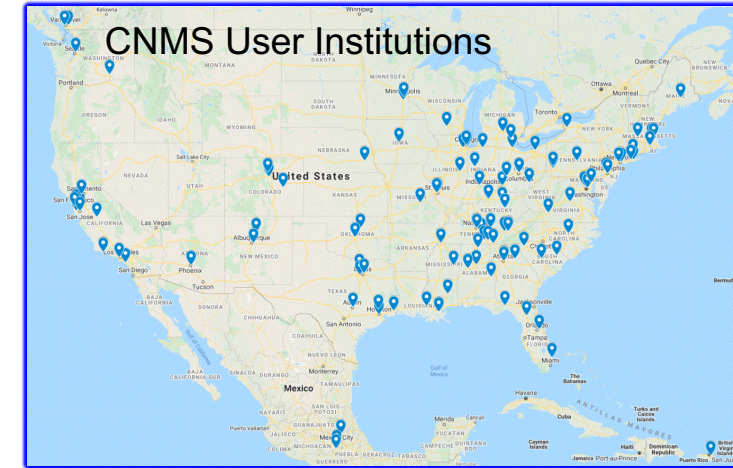 - Microelectronics Working Group (CINT)

- Monthly NSRC Directors Conference Calls
- Coordinated response to DOE requests
- Representation - BRN Workshops

U.S. DEPARTMENT OF **ENERGY** | Office of Science

3
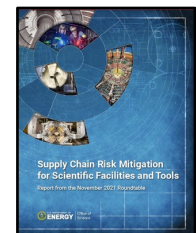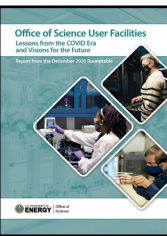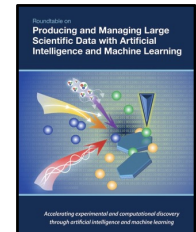
CNMS User Community

- Strengths:
  - Broad user base: ~60% of CNMS users are from outside the state of TN (~13% international); East/SouthEast regional strength
  - Remote access to many CNMS capabilities has enabled greater reach and demand
- Weaknesses:
  - Industrial users are low (4 active proposals) although industry participates on several proposals, despite targeted outreach
  - Lack of diversity, but increasing - user proposals from 10 HBCUs:
    - Alabama Agricultural and Mechanical University
    - Delaware State University
    - Elizabeth City State University
    - Fayetteville State University
    - Fisk University
    - Georgia State University
    - Howard University
    - North Carolina A&T State University
    - Tennessee State University
    - University of the District of Columbia

CNMS User Institutions

Locations of HBCUs

Geography presents OPPORTUNITIES to increase engagement with HBCUs

U.S. DEPARTMENT OF **ENERGY** | Office of Science

CNMS – Future Science Strategy

Complexity Develop new techniques for creating materials and structures

**Control** Use new techniques to explore materials properties

Infrastructure Investments being made to advance SC initiatives (microelectronics, QIS, AI/ML, clean energy)

Harnessing Complex Macromolecular Conformations
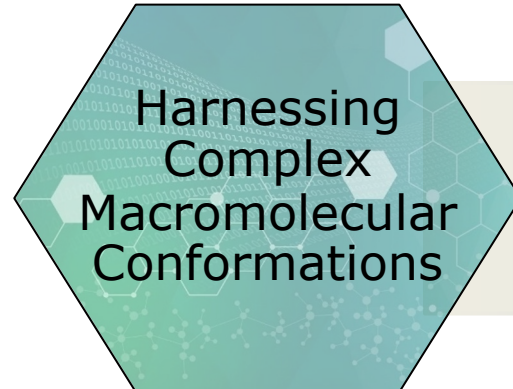
Understanding *structural and polarization dynamics* in polar polymers
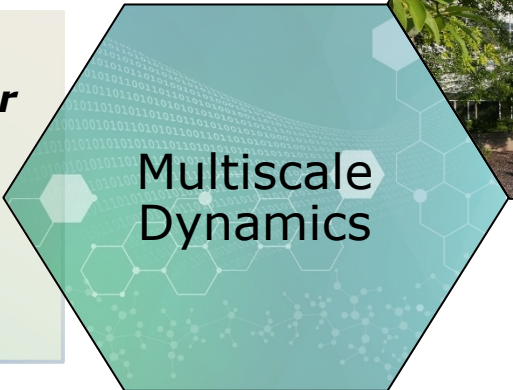
Develop materials design framework *for incorporating spatio-temporal dynamics* for on-demand materials functions

Multiscale Dynamics

Heterogeneities in Quantum Materials
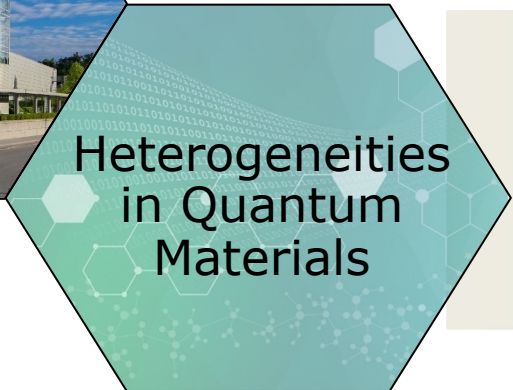
*Discovering, understanding, and controlling **quantum materials** behavior induced by heterogeneities*

Science portfolio underpinned by CNMS strengths in AI/ML (data analytics, autonomous experiments, etc.), theory, precision synthesis, and imaging (scanning probes, electron, ion)