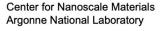
Synergy Between NSRCs and Co-located **Facilities/Inter-NSRC Collaboration**



Molecular Foundry Lawrence Berkeley National Laboratory







Center for Functional Nanomaterials **Brookhaven National Laboratory**

Gary Wiederrecht Center for Nanoscale Materials

October 29, 2024



Center for Integrated Nanotechnologies Sandia National Laboratories Los Alamos National Laboratory



Center for Nanophase Materials Sciences Oak Ridge National Laboratory















The NSRCs strategic scientific directions

Each NSRC has a strategic focus that defines science strengths



The NSRCs unique capabilities

Each NSRC has a strategic focus that defines unique, signature instrumentation



- Robotic nanomaterial synthesis by assembly
- In-situ and operando Xray and electron microscopy & spectroscopy
- Nanomaterial discovery by autonomous synchrotron X-ray scattering

- Metamaterials and nanophotonics
- Ion implantation from keV to MeV
- AI/ML and computational materials science (LAMMPS, MEMPHIS, NEXMD)
- Microelectronics and quantum device fabrication

- Hard X-ray Nanoprobe
- · Ultrafast imaging and spectroscopy
- Quantum materials characterization at ultralow temps
- Electron Microscopy (specifically dynamic imaging)



CNMS (ORNL)

- Ultrahigh-resolution STEM imaging and spectroscopy
- Atom probe tomography beyond conducting materials
- Cryo-EM for soft matter, biomaterials, and functional nanomaterials
- · Autonomous synthesis and characterization platforms



Foundry (LBNL)

- Electron Microscopy (specifically 4D-STEM)
- Accelerated Materials Discovery (robots, data, Materials Project, etc)
- Bio-inspired materials design and synthesis (peptoids etc)

All NSRCs utilize expertise in synthesis, characterization, nanofabrication, and theory and modeling















Examples of synergies and collaborations across the NSRCs

Between NSRC User Offices

- Monthly meetings between NSRC Directors and between User Program ٠ Managers
- Best practices most efficient and effective processes for running the ٠ centers
 - Reporting
 - Outreach •
 - User Meetings .
 - Data collection ٠
 - **Proposal Review Process** •
 - Adapt COVID procedures ٠
 - Promote remote users and self-driving labs ٠
- Set up and manage NSRC booth at conferences ٠
- Staff scientists participate on proposal review • committees

Scientific Proposals

- BES Renew A Collaborative Machine Learning Platform for • Scientific Discovery
- BES Renew A Digital Twin for In-Silico Spatiotemporally ٠ **Resolved Experiments**
- **Electron Distillery** ٠











ENTER FOR NANOPHASE









Synergies between NSRCs and Co-located User Facilities

- Collaborations with co-located facilities add uniqueness to our science and the capabilities that we can offer our users
- Examples of co-located facilities include DOE supported light sources (ALS, APS, NSLS-II) and the high-performance (HPC) computing facilities (ALCF, NERSC, OLCF)

CFN, CNM and MF are co-located with a Light Source

Enables operational partnerships, co-development of techniques, correlative imaging, collaborations on data handling, sample prep and analysis

CNM, MF and CNMS are co-located with an HPC

Collaboration on software infrastructure, AI-enabled workflows, data processing and curation



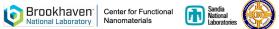


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Some specific project examples of collaborations and synergies!













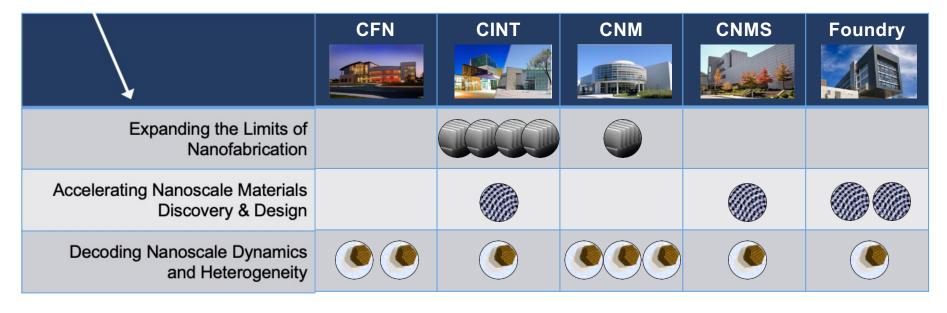






New equipment synergy example: NSRC recapitalization project

- NSRC-Recap fortifies capabilities in three nanoscience areas that will drive the next decade of discoveries
- NSRC-Recap is siting 17+ new instruments to align with NSRC strategic focus areas
- Brookhaven is the managing laboratory, with Chuck Black serving as the Project Director. Points of Contact at all 5 NSRCs meet at least weekly to discuss updates

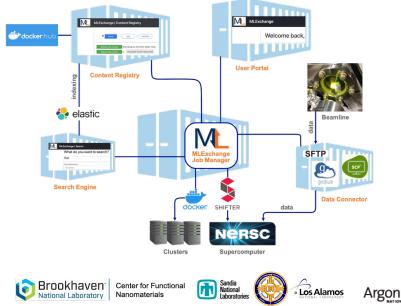




Software and data handling

Enhancements through collaboration between NSRCs and light sources

- MLExchange: Open-source software infrastructure and analysis tools shared across Foundry, CNM, CNMS and Light sources; enabling user accessible ML analysis pipelines
- Electron Distillery : Foundry-led, CNM, CFN + NERSC collaboration to process and visualize high rate (7 TB/min) data acquisition and develop ML tools



MLExchange

control computer on-site ¦ off-site high performance computing electron probe microscope processed beam data Perlmutter samp stage 100GE NERSC camera serve switch LBLnet 100 GE HAADF DAQ detector age strip pixelated detector event builder 12 x 10 GE ----4D Camera receiver servers 4 x 20 GE "Mothership 6" FPGAs

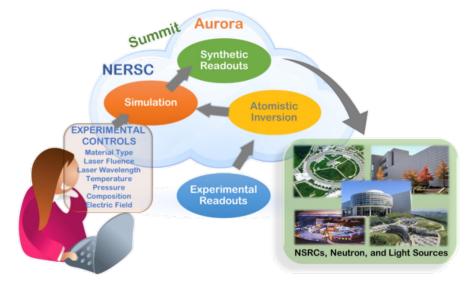
Electron Distillery

Direct connection of 100 gbps detectors to NERSC for on-stream processing



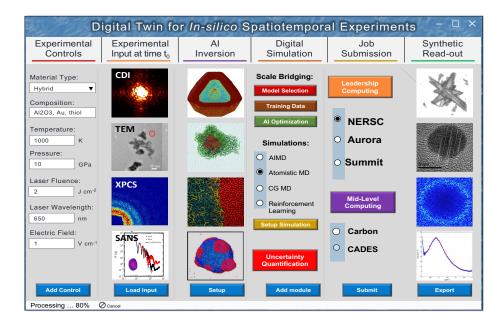
Digital Twin for Spatiotemporal Experiments

Enhancements through collaboration between NSRCs and light sources



- Al solutions to the inverse problem, i.e., information extraction from time-resolved experiments
- AI/ML Guided multi-fidelity bridging for physically accurate & efficient dynamical simulations
- Shared workflows for seamless information exchange between models and experiments





Collaboration Across Scientific User Facilities: CNM, CNMS, MF, CFN, CINT, APS, ALS, SLAC

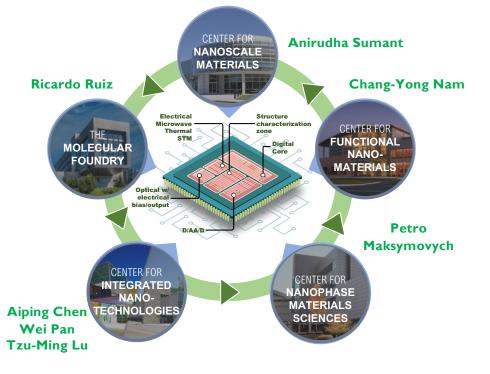




Cross-NSRC working groups to address national priorities

Example: Microelectronics

Collective resource to accelerate CHIPS and Science Act innovation and economic impact



Industry and University Research Needs

- Metrology, Modeling and AI for 3D Heterogeneous Integration
- Materials Synthesis
- Integration of Non-Conventional Materials and Device Architectures
- Tools for Next-Generation Lithographic Patterning
- Advanced In-Situ / Operando Characterization

Combined Capabilities, Expertise, and Facilities

- **40,000 sq. ft. of flexible, fast-turn cleanrooms** for nanofabrication and integration of early stage materials, devices and architectures
- More than **100 materials synthesis laboratories** for inorganic, organics, and hybrid composites
- More than **30 unique measurement capabilities** for metrology, property, performance, and in-situ / operando studies
- Atomic to microscale modeling tools, including AI/ML for Lab to Fab correlations
- **Portal to other DOE** Facilities and User Facilities

Other NSRC working groups: quantum information science, data science AI/ML, clean energy





Conclusion: NSRC synergies and co-located facilities lead to increased collaboration and impact



Connecting to national priorities, the NSRCs successfully collaborate as well as operate and co-develop scientific capabilities with the DOE light sources, the HPC resources, the neutron sources and NNSA facilities

There is a strong synergy between NSRC science and other DOE facilities; clearly emphasized by co-location

We look forward to future great partnerships !







