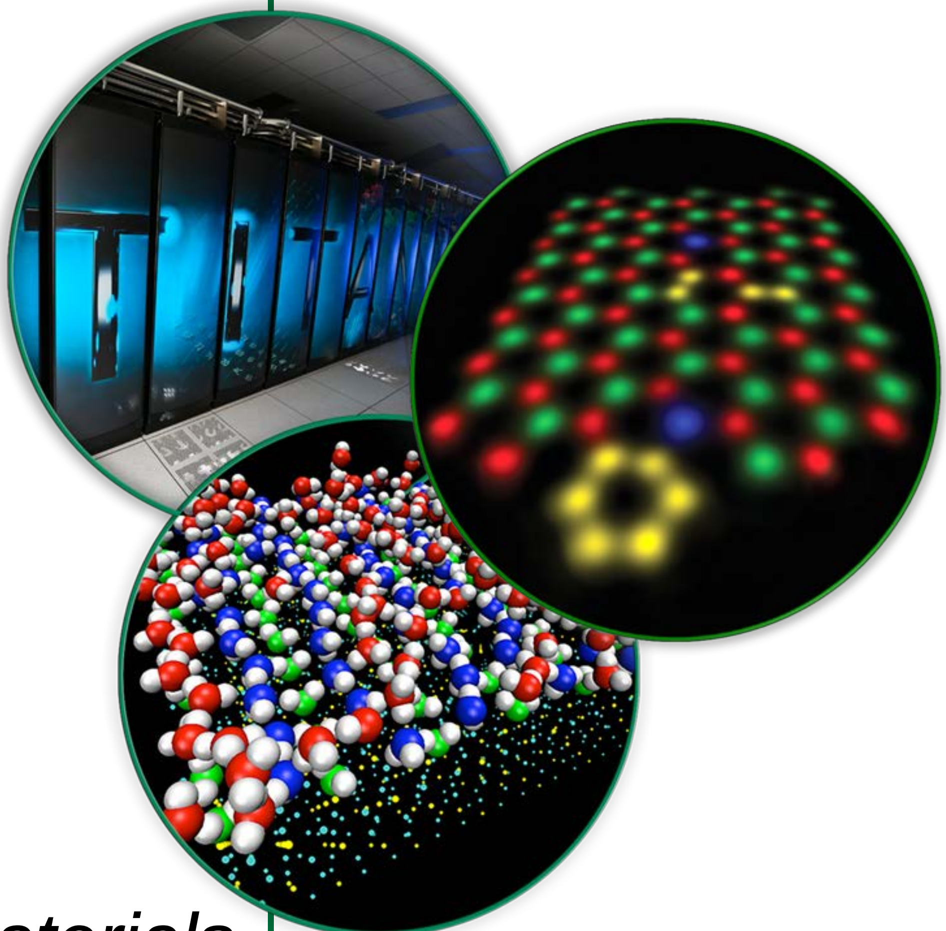
Institute for Functional Imaging of Materials (IFIM)



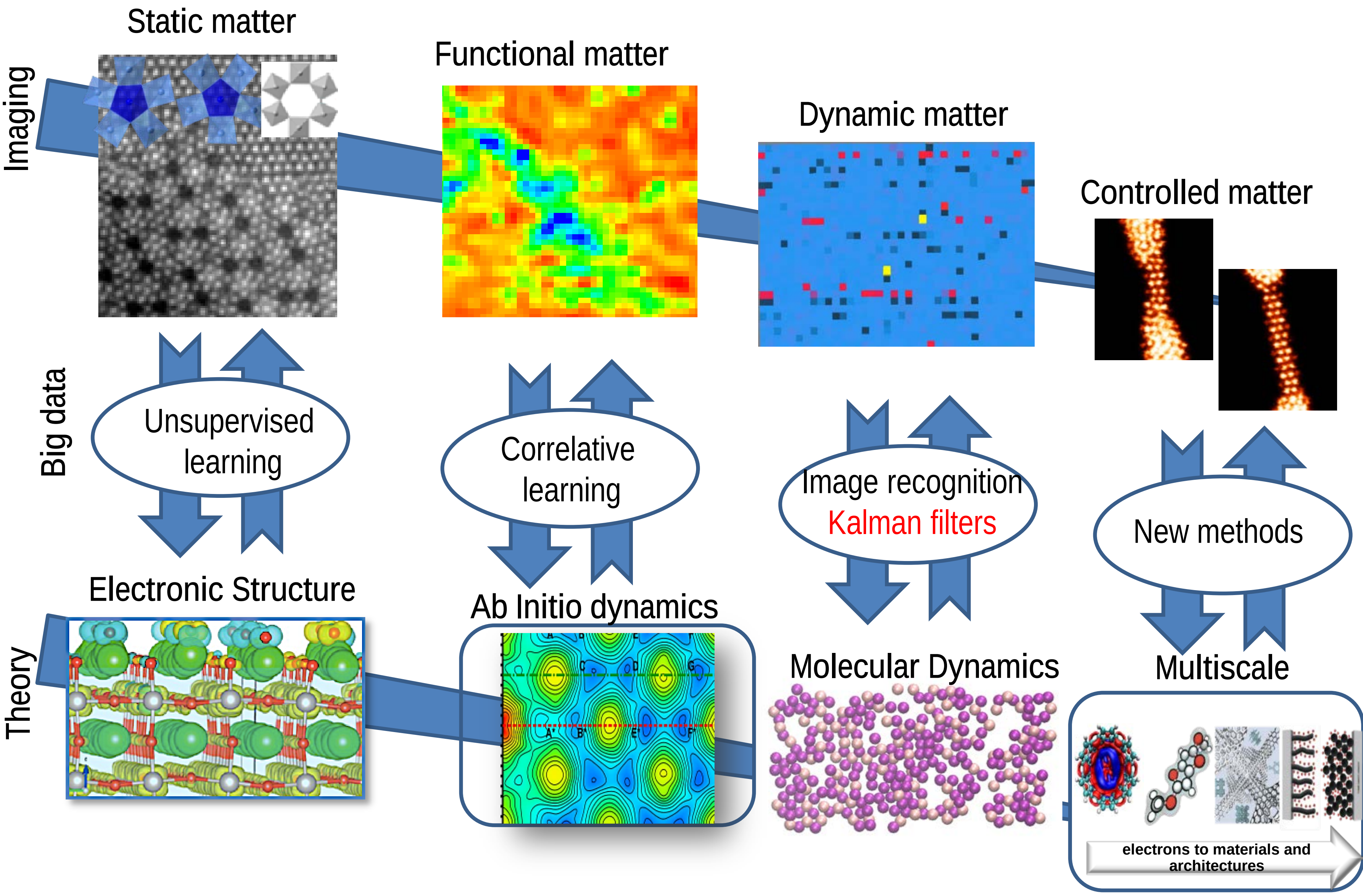
Sergei V. Kalinin

Guiding the design of materials tailored for functionality

U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Dynamic matter: information dimension



Imaging: The big picture

Our scientific paradigm is shifting from the classical concept of *synthesis-characterization-theory-computation* to include *data mining, correlative functional imaging, and local theory-experiment matching* of multi-dimensional (multi-modal), spatially and temporally resolved information

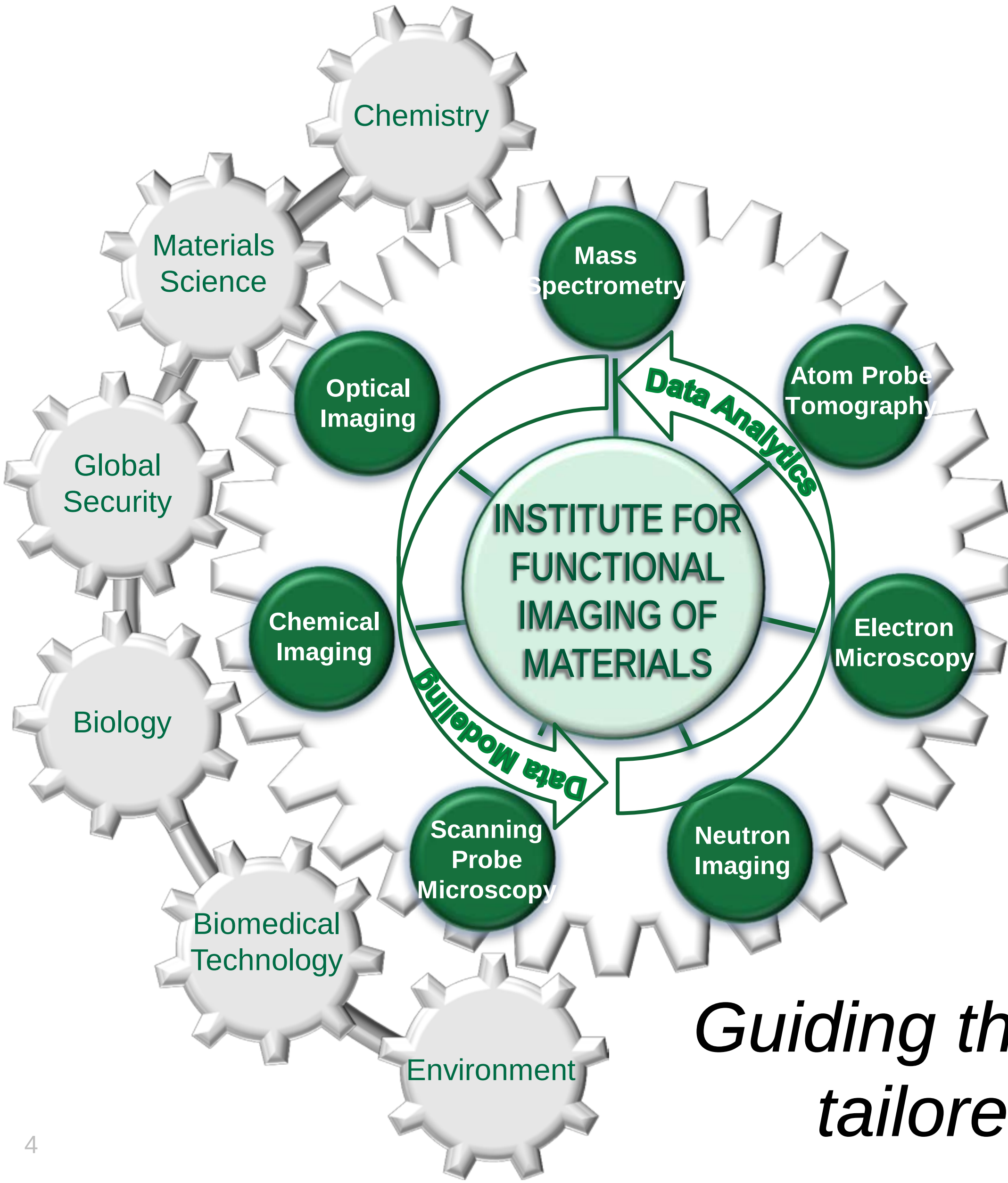
ORNL has unique strengths in:

- Physics and chemistry on the atomic scale in real space
- Mesoscale structure and functional probing
- Big data and predictive theories: biggest computation effort

Now is the time to bridge **physical imaging** with **theory** via **big data and data analytics**

Advancing the Science and Technology of Imaging

ORNL's Institute of Functional Imaging of Materials



Goals:

- Coordinate imaging development effort across groups, divisions, directorates
- Strengthen imaging framework to overcome barriers for entering new research areas
- Enhance the core strengths of imaging programs, including facilities and instrumentation, and identify strategic needs
- Foster synergy between imaging programs and establish critical links with computational sciences and theory
- Tap into collective imaging expertise to offer imaging solutions
- Identify high priority areas for imaging related research

Guiding the design of materials tailored for functionality

OAK RIDGE National Laboratory

Physics from atomic scale images

- 1912 – Laws of Diffraction (Braggs)
- Pair correlation functions: average atomic positions, site compositions, thermal vibrations
- Shaped the way generations of physical scientists think
- Many systems do not comply to simple symmetry-based descriptions: nanoscale phase separations, morphotropic systems, quazicrystals, spin and cluster glasses

Opportunities for atomic imaging:

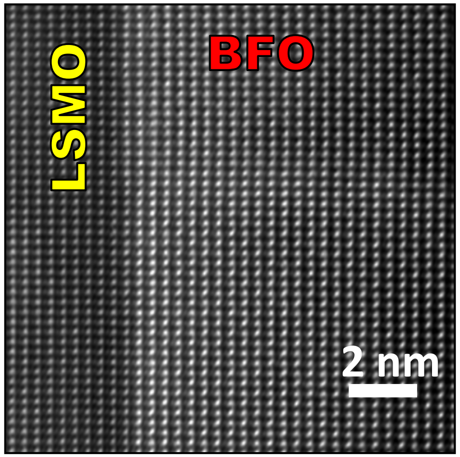
- Structure beyond scattering
- Structure-property correlations on single atom level
- Integration with predictive theory

Atomic scale: beyond scattering

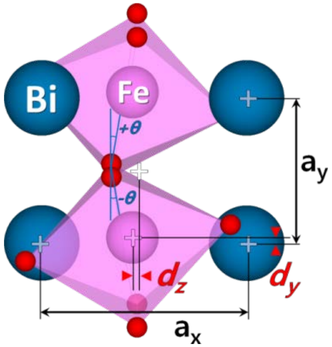
Level 0:
Illustration

- Two materials
- Sharp coherent interface
- Higher atomic number to the right

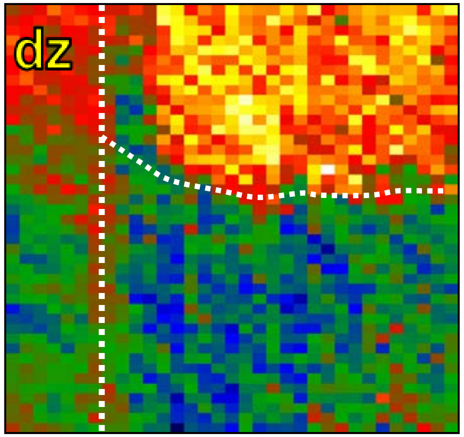
Z-contrast STEM



Level 1:
Atomic positions

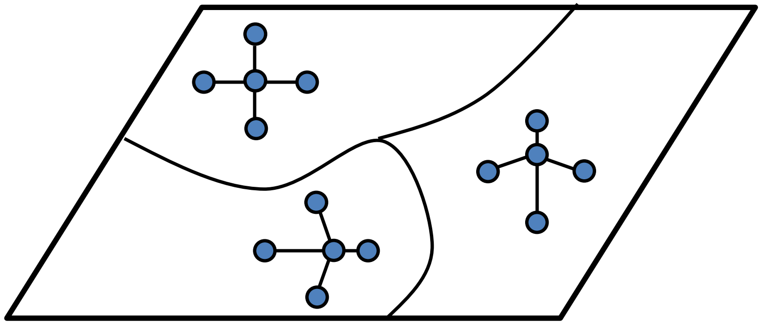


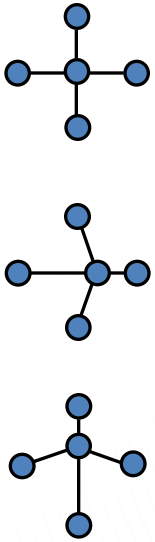
Polarization map



- Two ferroelectric domains
- Bent domain boundary

Level 2: Local Analysis





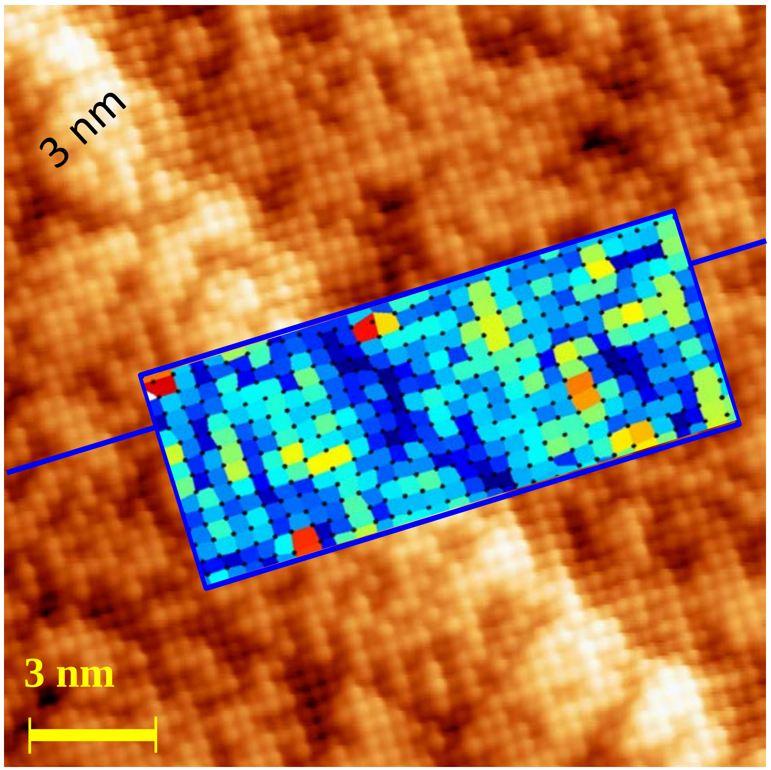
Phase I

Phase II, orientation 1

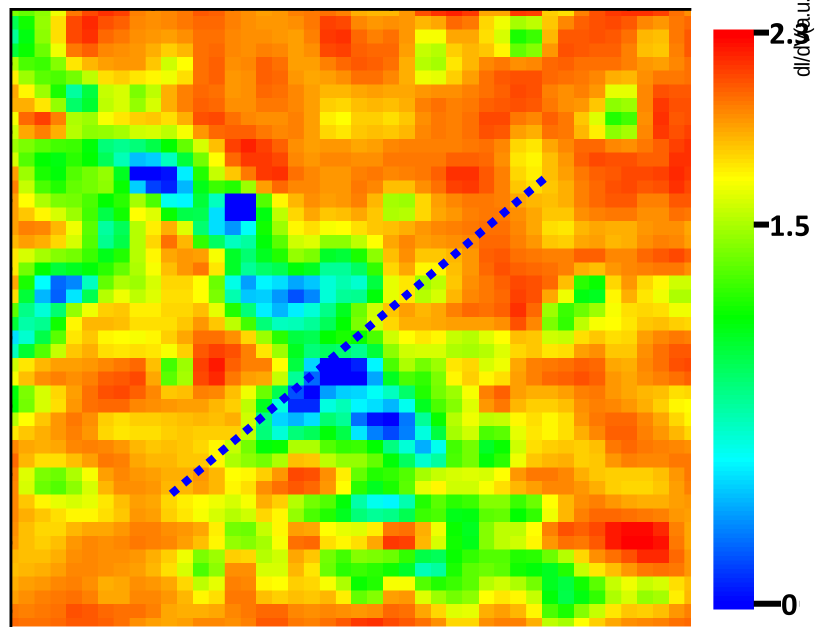
Phase II, orientation 2

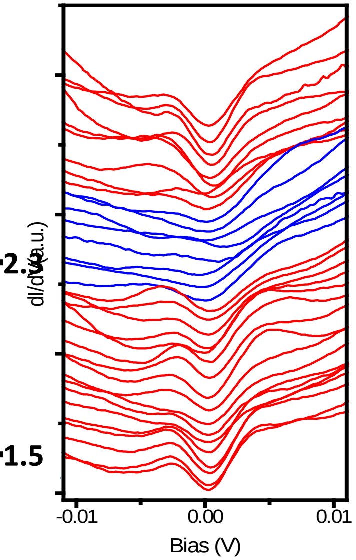
Next step: local structure-property relationships

STM image of (11) at L-He



Superconductive gap map

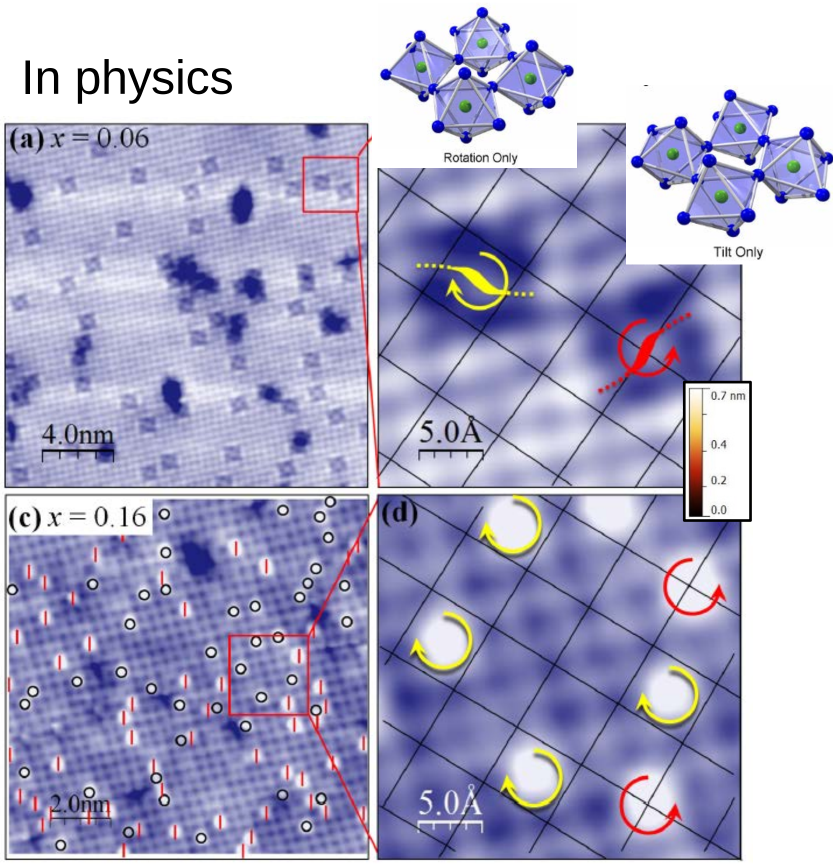




The defect preserves lattice continuity, but is associated with change in molar volume and lattice parameter - Guinier-Preston zone. Superconductivity is suppressed at the defect.

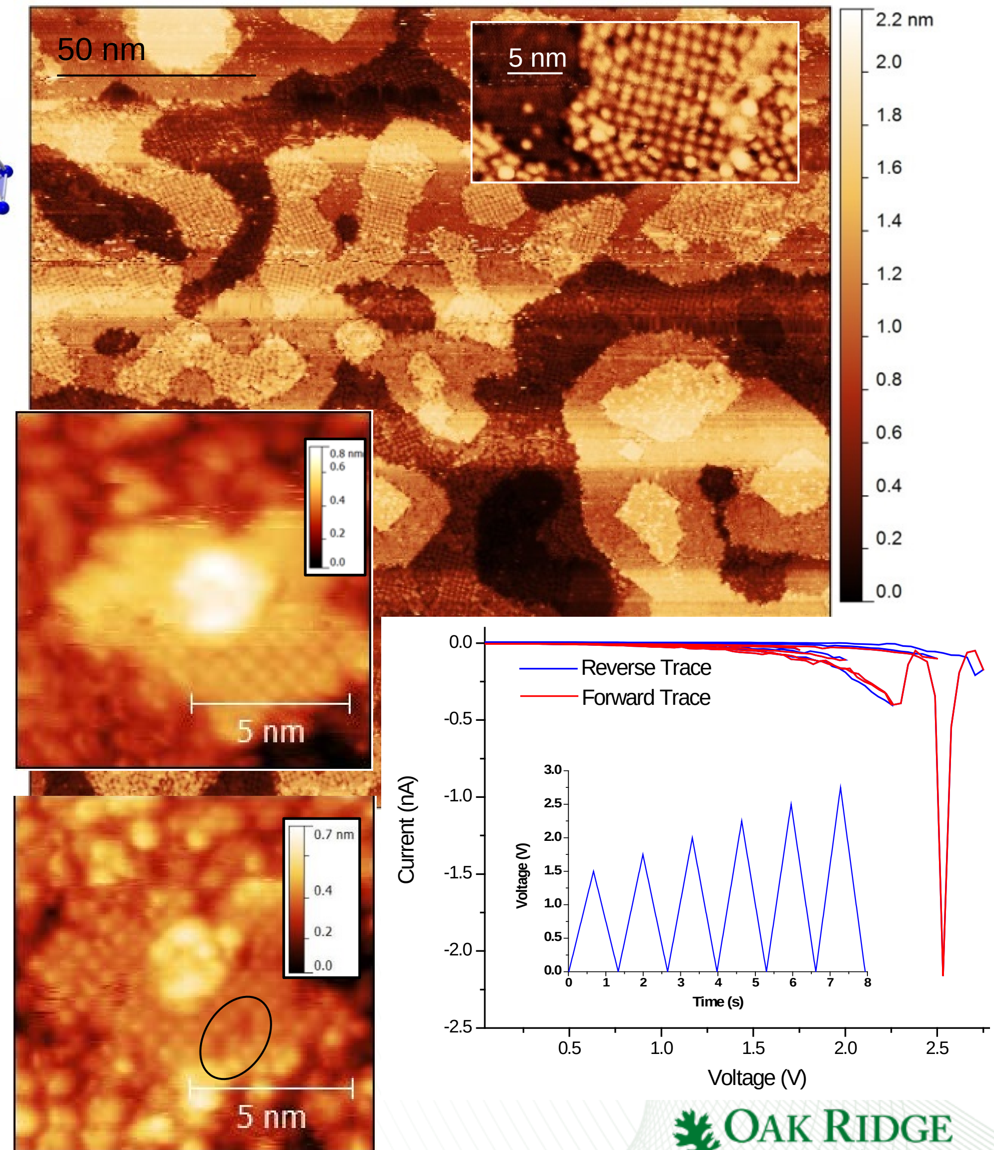
Next step: local structure-property relationships

In physics



Mn atoms in layered ruthenate
Sci. Rep. 2013

… and chemistry



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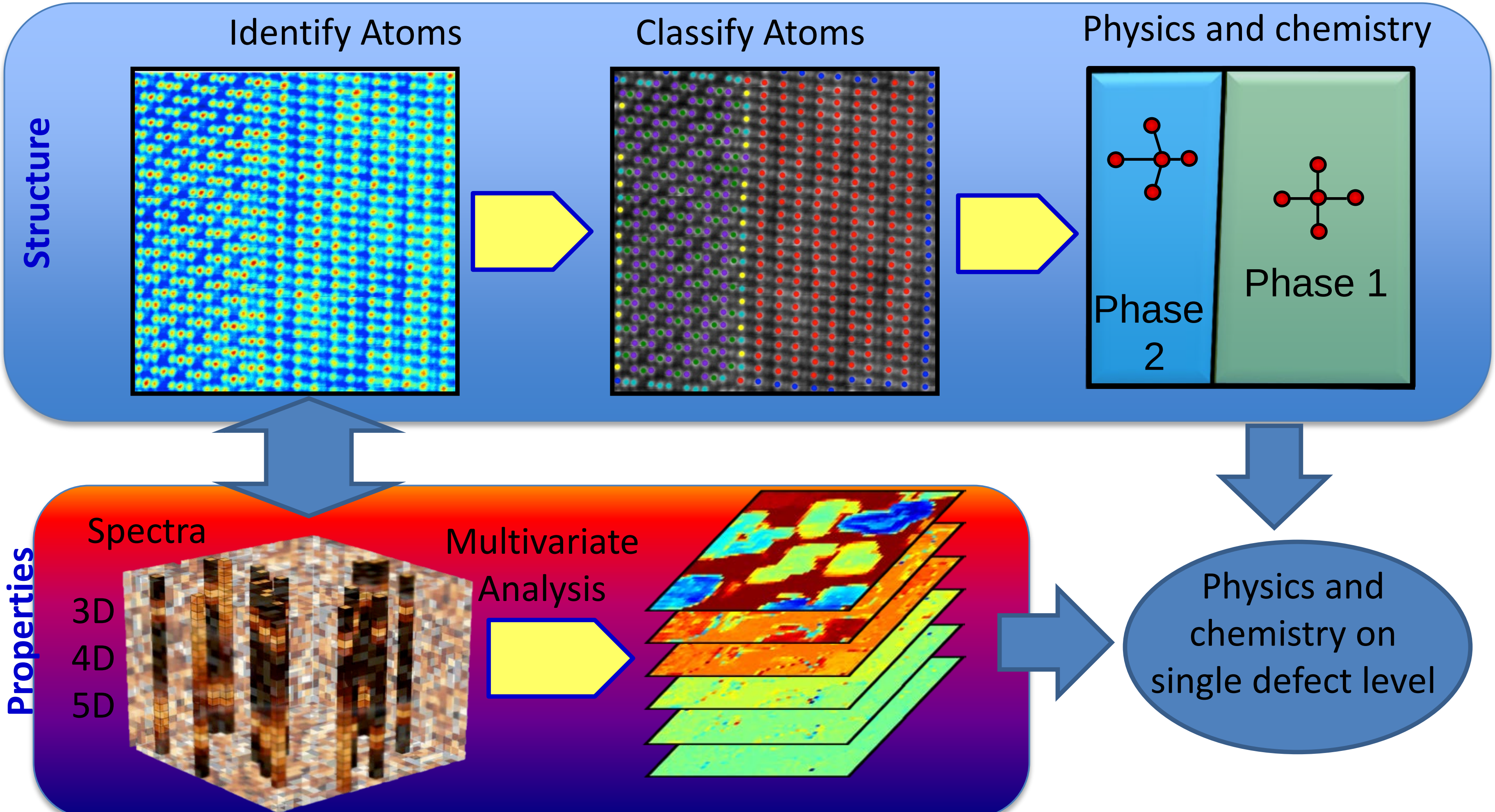
Big data: Atomic-Scale Structure and Functionality



Need new language:

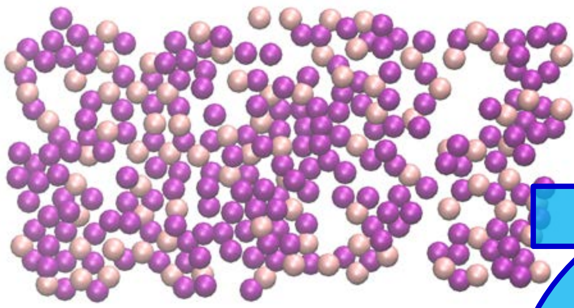
1. What are structural descriptors?
2. How do we define local symmetry, phases and ferroic variants?
3. How do we introduce and quantify translational symmetry?

What do we learn:

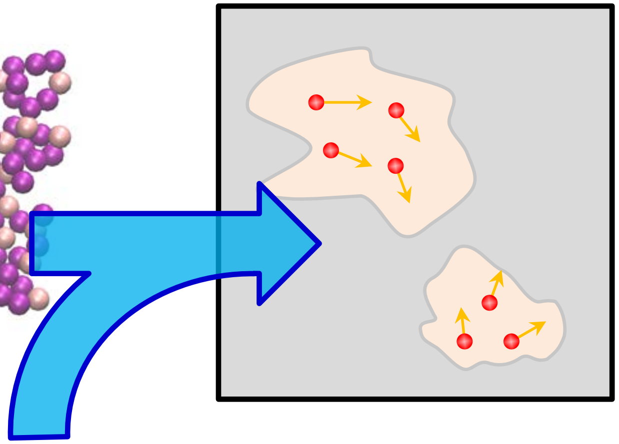
1. Structure-property relationship on single atom, molecule, and defect level
2. Feedback to theory through microscopic degrees of freedom
3. Input to Materials Genome

Deep Data: Exploring Local Degrees of Freedom

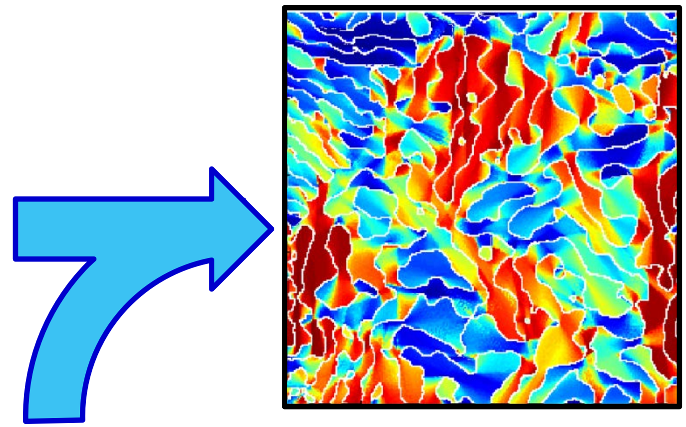
Atomistic simulation



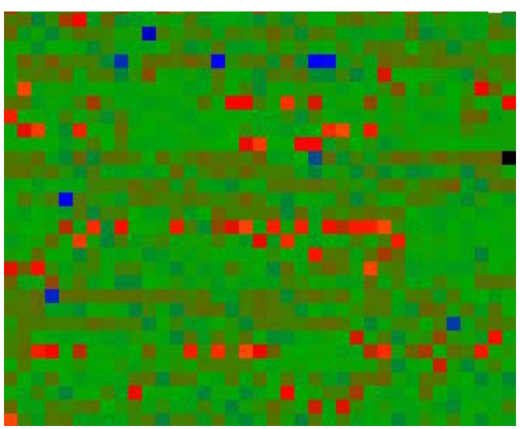
Coarse Graining

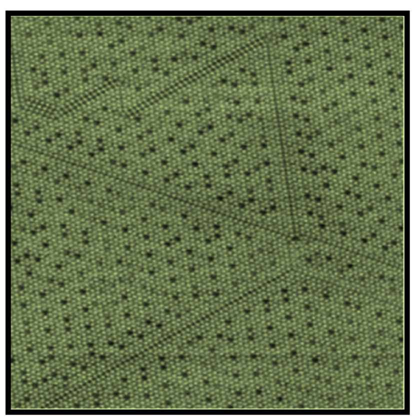


Mesoscale simulation

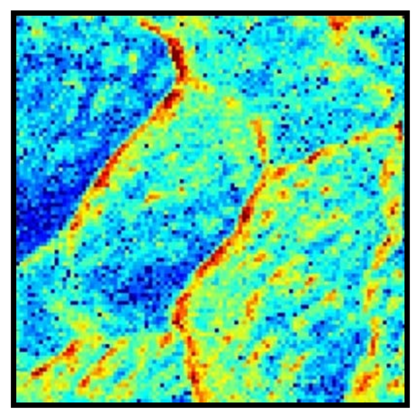


Atomistic Imaging



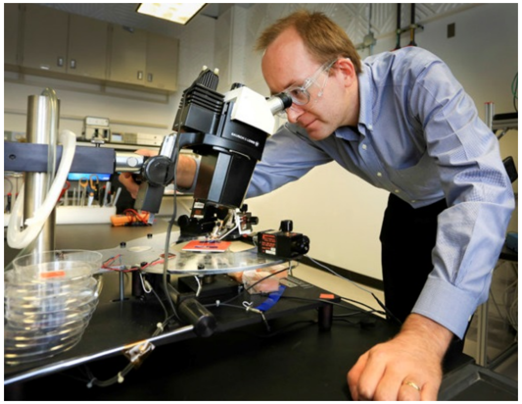


Mesoscale Imaging



Smart Data: From Human to Automatic Systems

Expert



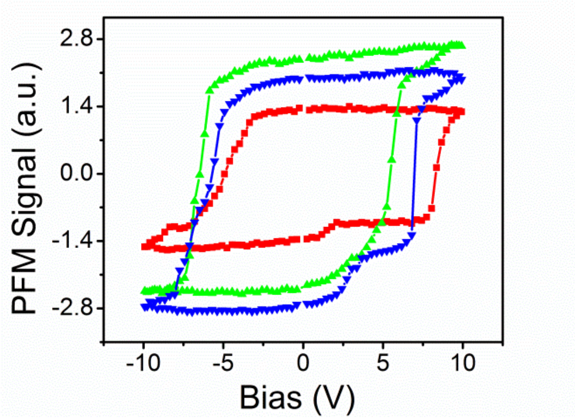
Control

Decision making

Automatic Expert System

User Model

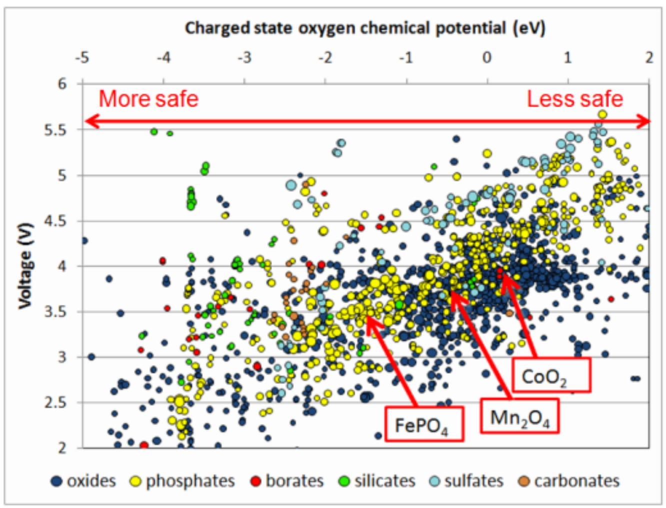
Experimental data



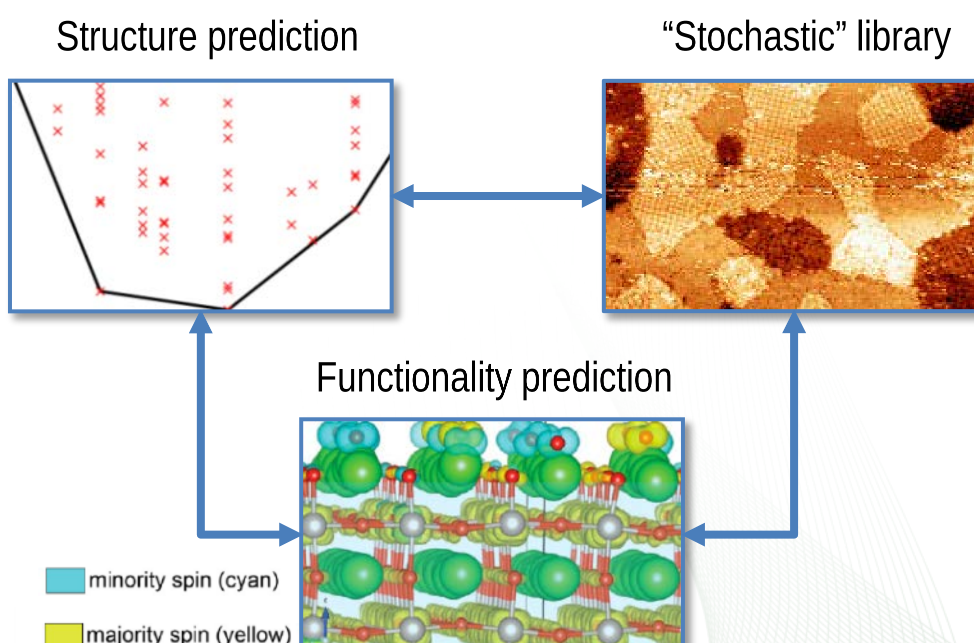
- Synthesis of expertise
- Routine analysis
- Identification of anomalies
- Initial training of new practitioners

Shifting scientific paradigm

- **Classical scientific method:** Observation → Hypothesis → Verification
- **Big data in theory:** new opportunities for science (e.g. Materials Genome)
- **Structural + functional Imaging:** big data in experiment



Direct matching: large scale computation and experimental probing



ACS Nano 7, 4403 (2013)

Imaging Challenges

Imaging challenges

- **Challenge 1:** Can local structures be measured in time and space, and be correlated with macroscopically-averaged functional behaviors?
- **Challenge 2:** Can local functional properties be probed and manipulated, and can this knowledge be extrapolated to macroscopic assembly scales?
- **Challenge 3:** Can we establish the link between local structure and functionalities and predictive theories on the level of microscopic degrees of freedom?

ORNL Institute for Functional Imaging of Materials (IFIM) will provide the pathway to address these challenges through integration of multimodal imaging techniques with big- and deep data analysis

Imaging: Physics, chemistry, and materials science on atomic scale

- For 100 years atomic structure of matter has been available only through scattering
- The progress in electron and scanning probe techniques now enables determination of atomic positions with better than 10-pm precision
- Associated spectroscopies provide insight into local functionalities on single molecule, defect, and bond level

How do we collect, combine, systematize, and interpret this data and integrate it with predictive theory?

Imaging: The challenge of mesoscale

- Neutron and X-ray tomography yields unprecedented view of structure and chemistry of hard, soft, and living matter in 3D, often dynamically.
- Establish synergy between atom probe effort and ORNL's core strengths in materials and other areas of structural and functional imaging
- Integration of imaging data from multiple channels/techniques (e.g. neutrons + XRD, atom probe + (S)TEM, tomographic information + high resolution 2D data)

How do we analyze multimodal 3D structural data and link it to macroscopic functionalities?

Imaging: Chemical imaging

- How do we develop probes for specific aspects of chemical, electrochemical, and biological functionality,
- How do we develop and enable appropriate instrumental platforms, and improve their resolution
- Applications to artificial and stochastic combinatorial libraries

How do we combine data of different nature, from multiple imaging sources and differing length scales

Why ORNL

IFIM: why ORNL

- **World leading electron microscopy effort:** uniquely qualified staff and cutting edge tools, and have the opportunity to tie it in in unique science- and information driven program
- **One of the biggest SPM groups in North America:** unique opportunities to link to chemical imaging and chemical detection modes
- **Neutron imaging and Atom probe:** Opportunity to tie to basic physical and biological sciences

- World-class computation science effort
- Big data and analytics: biggest computation effort in DOE

Imaging at ORNL

- Physics from atomic scale images: probe and electron microscopy (*A. Borisevich, MST*)
- Describing the mesoscale: energy and information dimensions (*S. Jesse, CNMS*)
- Chemical imaging: from structure to functionality (*O. Ovchinnikova, CSD*)
- Neutron imaging (*H. Bilheaux, SNS*)

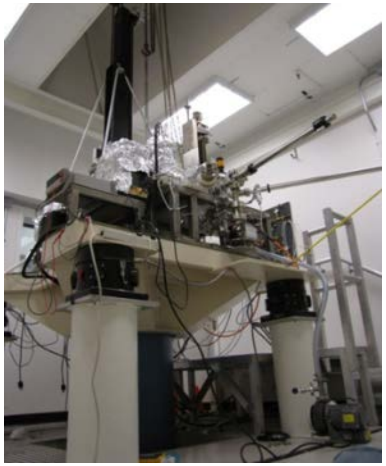
Big data:

- Machine learning
- Genetic algorithms
- Image analysis

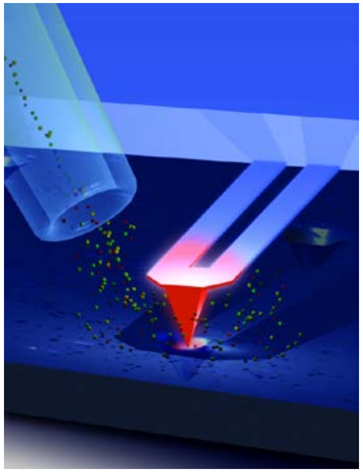
Theory:

- DFT
- MD
- Phase field

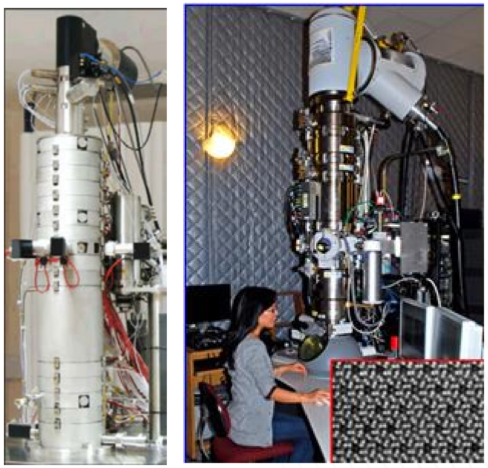
Probe Microscopy



Chemical imaging



Electron Microscopy



Neutron Scattering

Harnessing predictive power through computational materials science

- Over the past decade, computing power has increased by a factor of 1,000
- In the same period, software advances have added another factor of 1,000 for many applications
- This million-fold increase provides access to length scales, time scales, and numbers of particles that transform our ability to understand and design new materials
- This has profound implications for the pace of discovery and the creation of new technologies

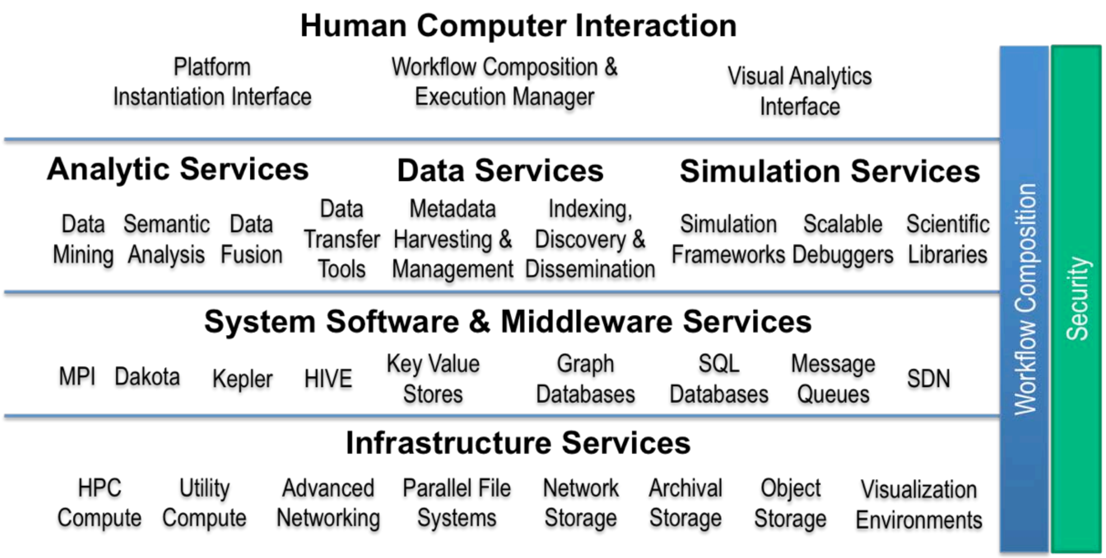
ORNL’s 27-petaflop supercomputer

CADES

Compute & Data Environment for Science

- A diverse computing and data ecosystem
- Matrix staff with expertise in computing and data science
- Focused on the technical computing needs of the scientific and engineering R&D communities across ORNL
- Supporting many projects today across ORNL

Expert Services



Infrastructure