Argonne Integrated Imaging Initiative: the Sum is Greater Than the Parts

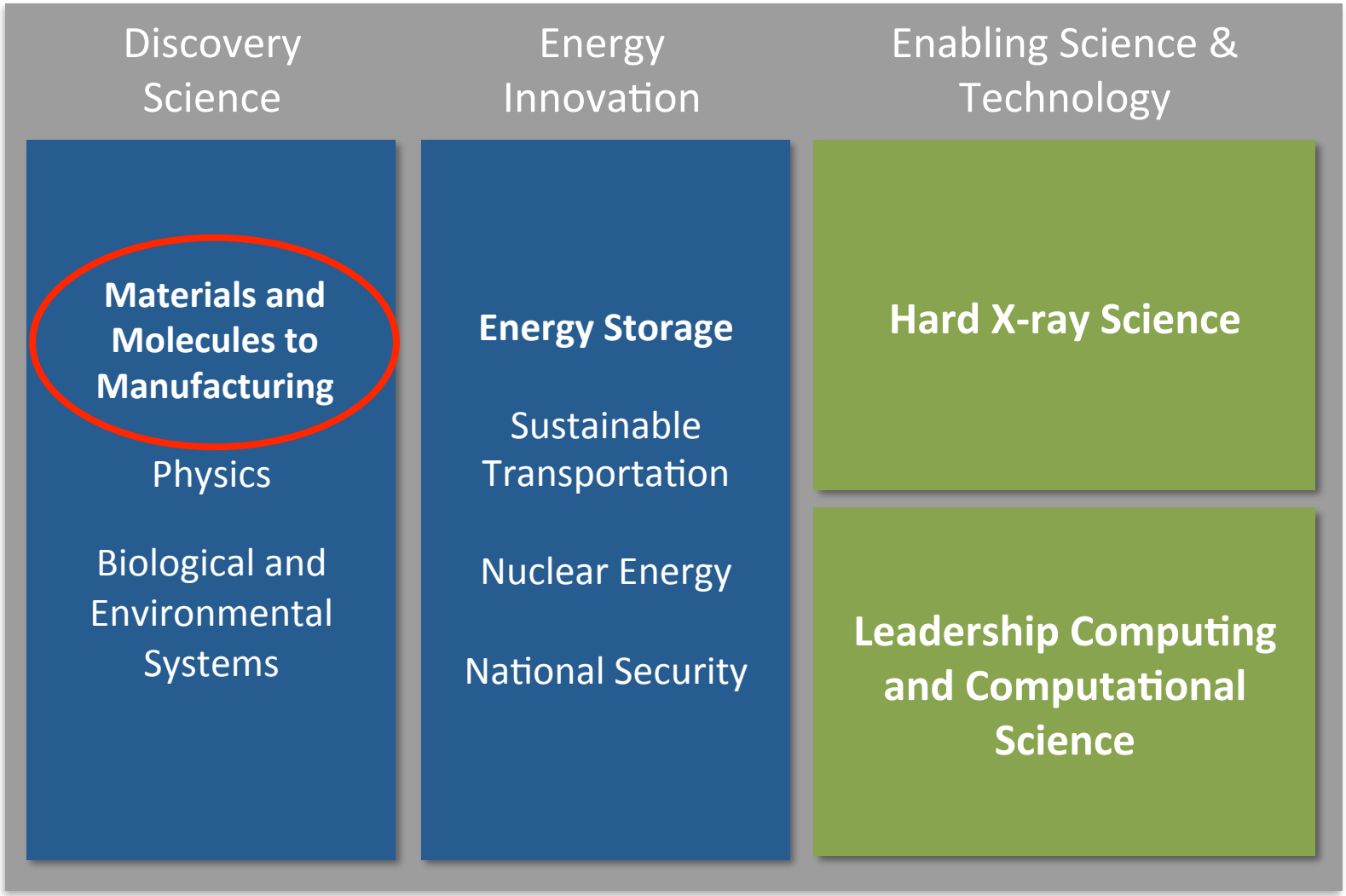
Ian McNulty

Center for Nanoscale Materials, ANL

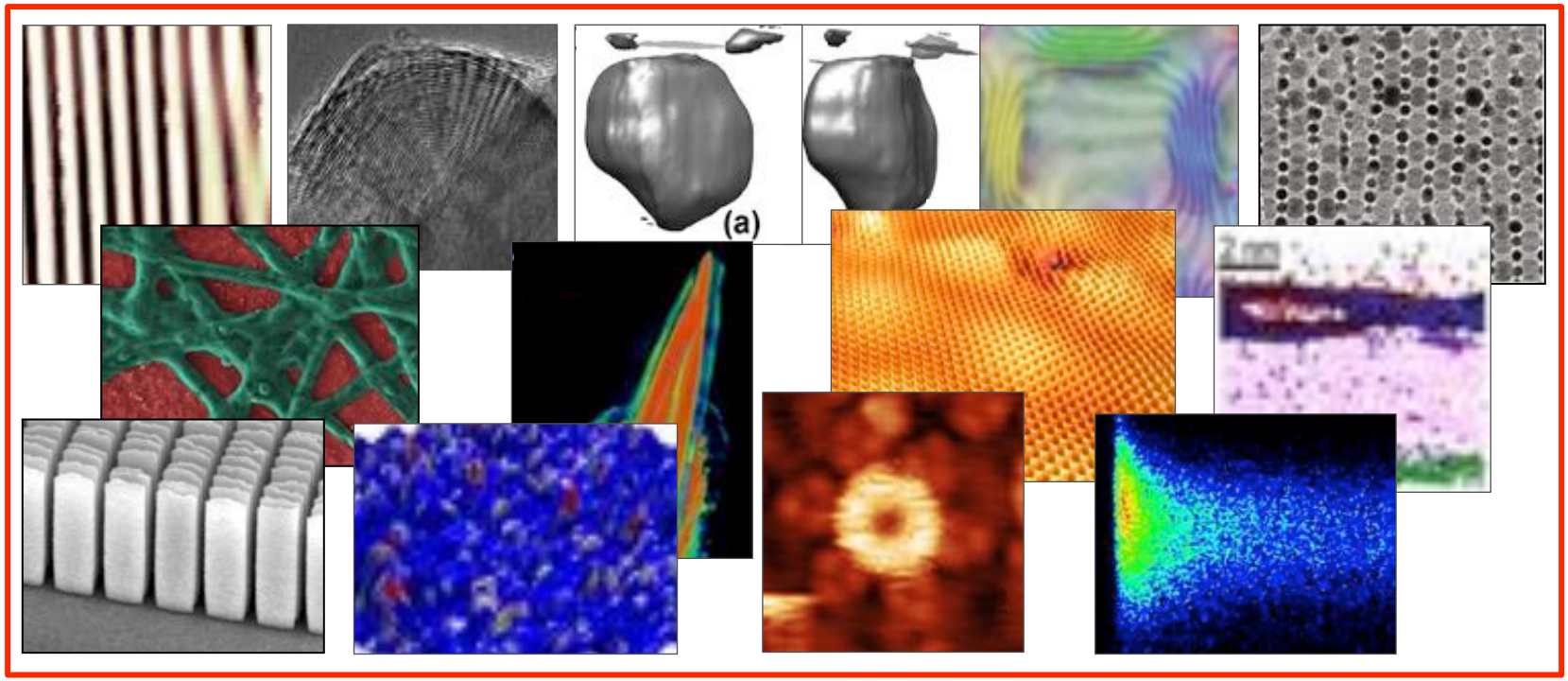
Oak Ridge National Laboratory

8 June 2015

Argonne's major strategic initiatives



Integrated Imaging Initiative (I^3): A Complete View of Nature



Understand and control the behavior of materials by probing and visualizing behavior in response to external stimuli over multiple temporal and spatial scales

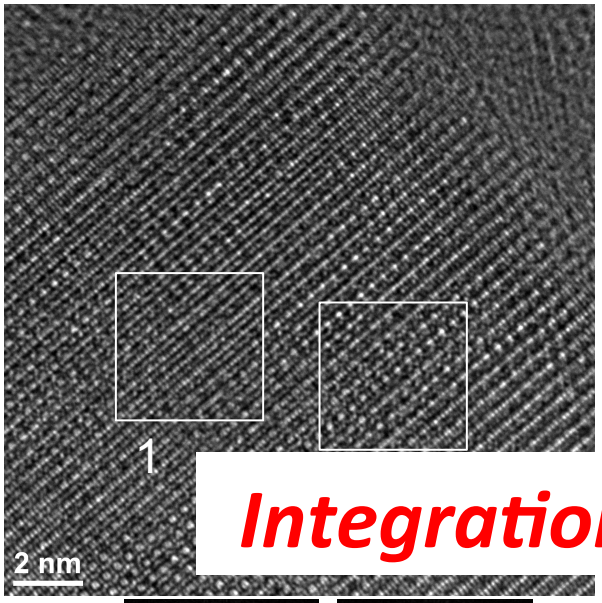
www.anl.gov/imaging

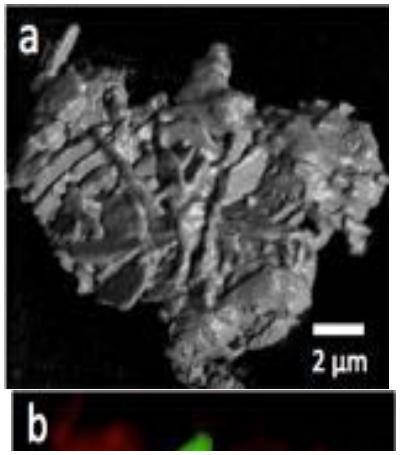
Hierarchical understanding of batteries

Sub-nm resolution

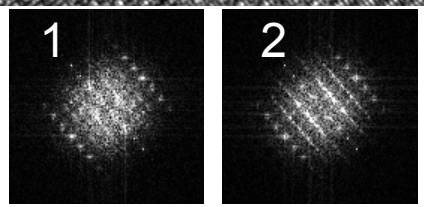
Few 10s nm resolution

Micron and sub-second resolution



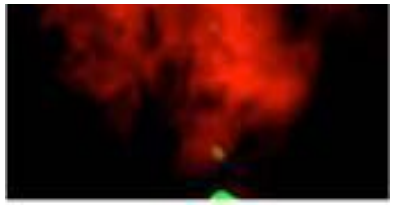


Integration of Imaging Data is Needed!



High-resolution TEM image of Li- and Mn-rich $0.5Li_2MnO_3 \bullet 0.5LiCoO_2$ composite electrode material.

Local diffraction information shows different ordering in two marked regions.



(ABR-1 (+):$Li_{1.2}Mn_{0.55}Ni_{0.15}Co_{0.1}O_2$) electrode during charge cycling .

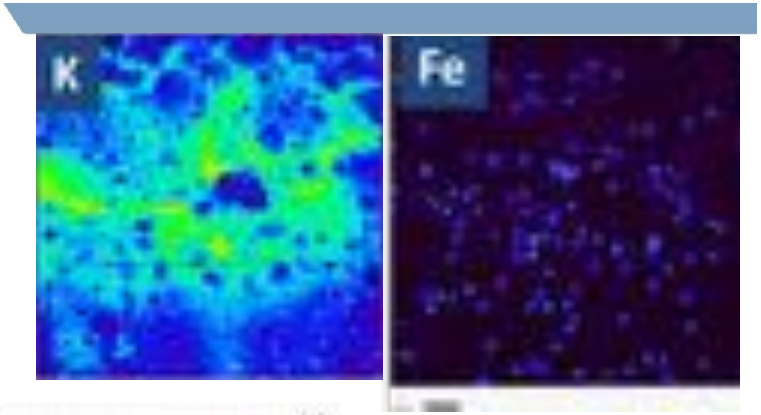
Top: 3D structure by x-ray nanotomography.
Bottom: Mn density distribution by scanning x-ray fluorescence.

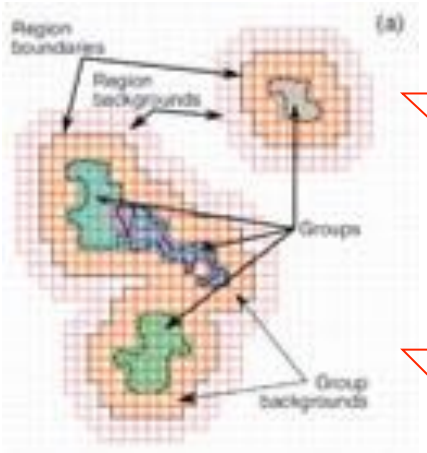
X-ray microtomography is used to compare the surface-volume ratio of different Cu/Sn battery electrodes during in-situ operation

J.G. Wen, D. Miller (EMC), R. Winarski, V. Rose (CNM), F. Brushett (MIT), L. Trahey, J. Vaughey (CSE), N. Chawla (ASU), X. Xiao (XSD)

The science of "data"

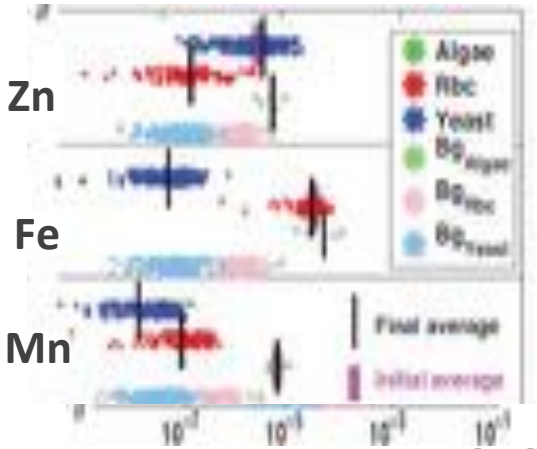
- Today
  - Manually moving and analyzing data
  - Ad hoc tools that do not scale to the next generation of instruments
  - Many algorithms are “dangerous” if not used carefully
- Tomorrow
  - Extensive toolset of scalable algorithms (e.g., machine learning, statistical)
  - Scientific knowledge integrated with analysis, visualization and simulation
  - Automatic integration of data from multiple sources, cataloguing and transfer via Globus tools
  - Efficient data reduction strategies





Identification and Classification

Reduction and Visualization



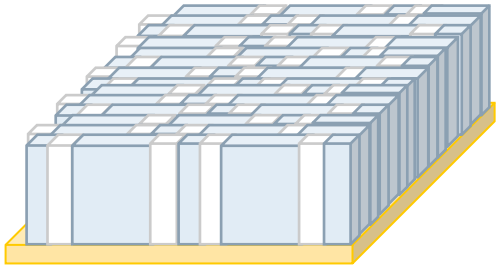
Elemental content [ng]

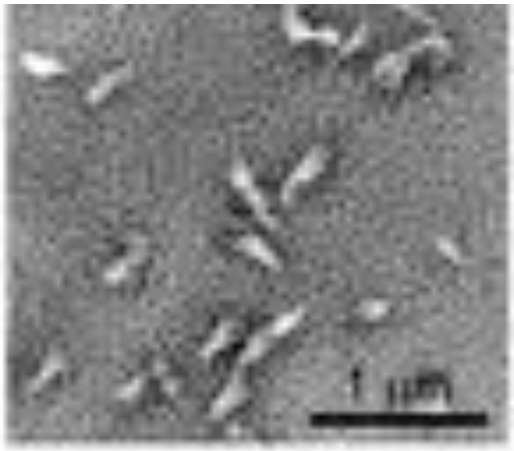
***Top**: X-ray fluorescence maps of different cells.*
***Middle**: Software automatically identifies and classifies 3 different cell types, enabling further analysis.*
***Bottom**: Comparison of resulting average elemental content per cell*

S. Wang, JSR 21, 568 (2014)

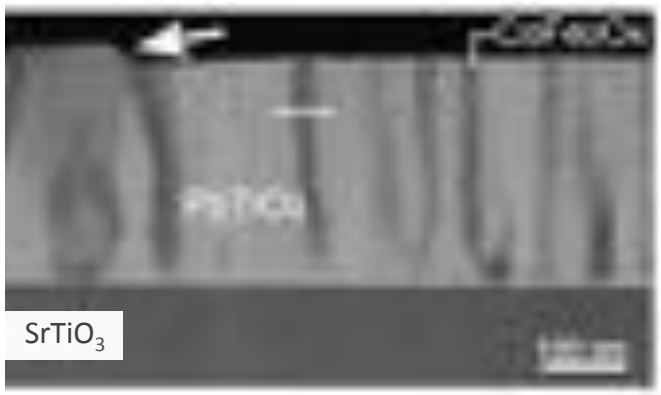
Self-assembled $CoFe_2O_4$ -$PbTiO_3$ multiferroic nanocomposites

- Self-assembled $CoFe_2O_4$–$PbTiO_3$ nanocomposites deposited on $SrTiO_3$ by metalorganic chemical vapor deposition (MOCVD)
- Vertical architecture allows for increase in interfacial surface area and increased interfacial magnetoelectric interactions

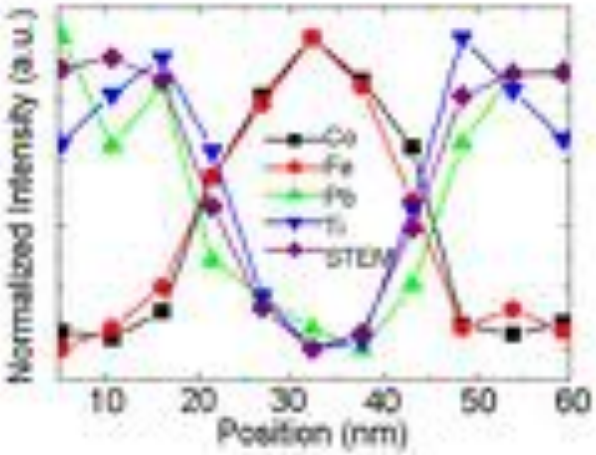




SEM image of surface



STEM-HAADF cross-section image

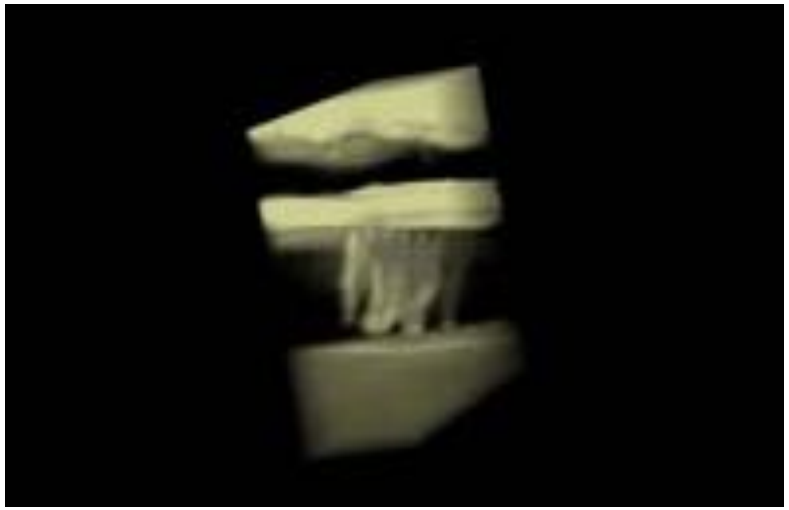


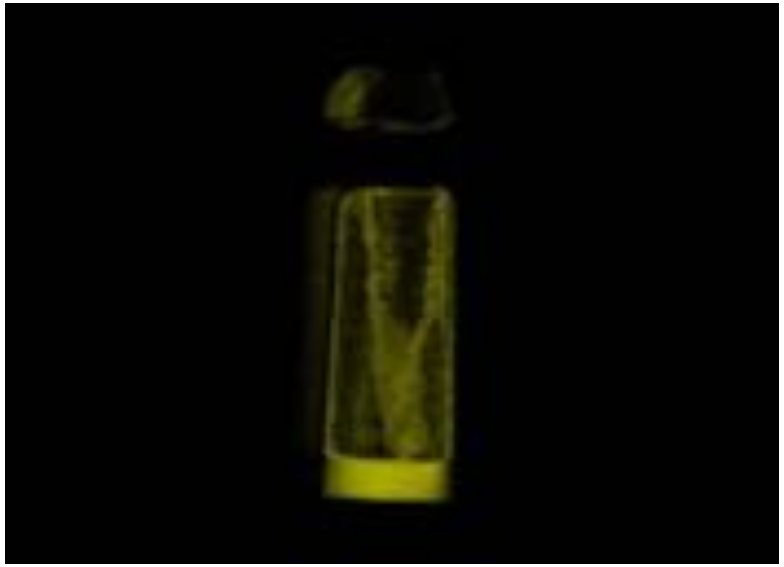
Normalized EDS elemental profile recorded at white line in STEM image

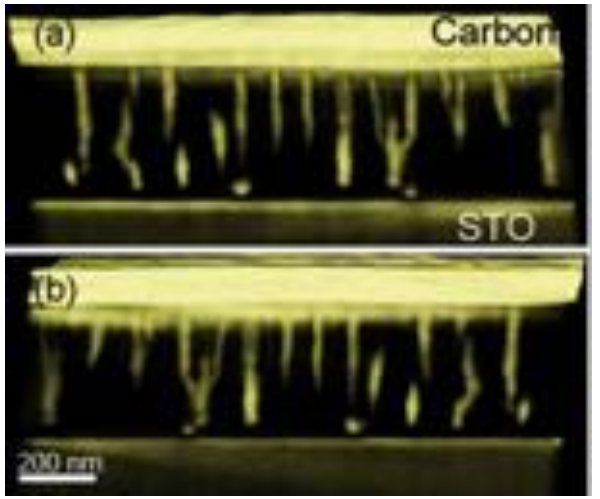
- CFO forms filaments in a PTO matrix with large PTO grains of different orientation.
- The microstructure controls the piezoelectric domain configuration and magnetic anisotropy.

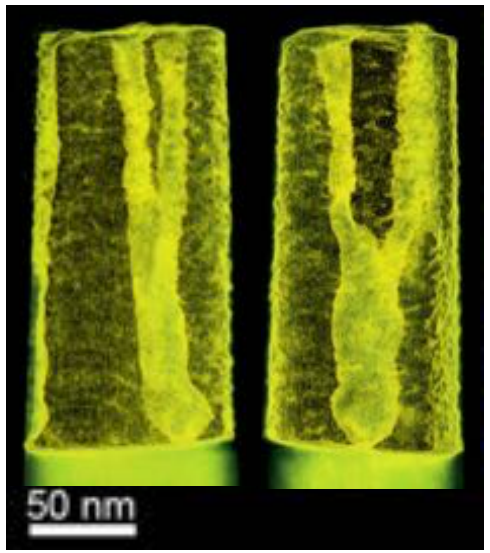
M. Pan, JAP 110 034103 (2011)

Multiferroic nanocomposites: CFO grain structure





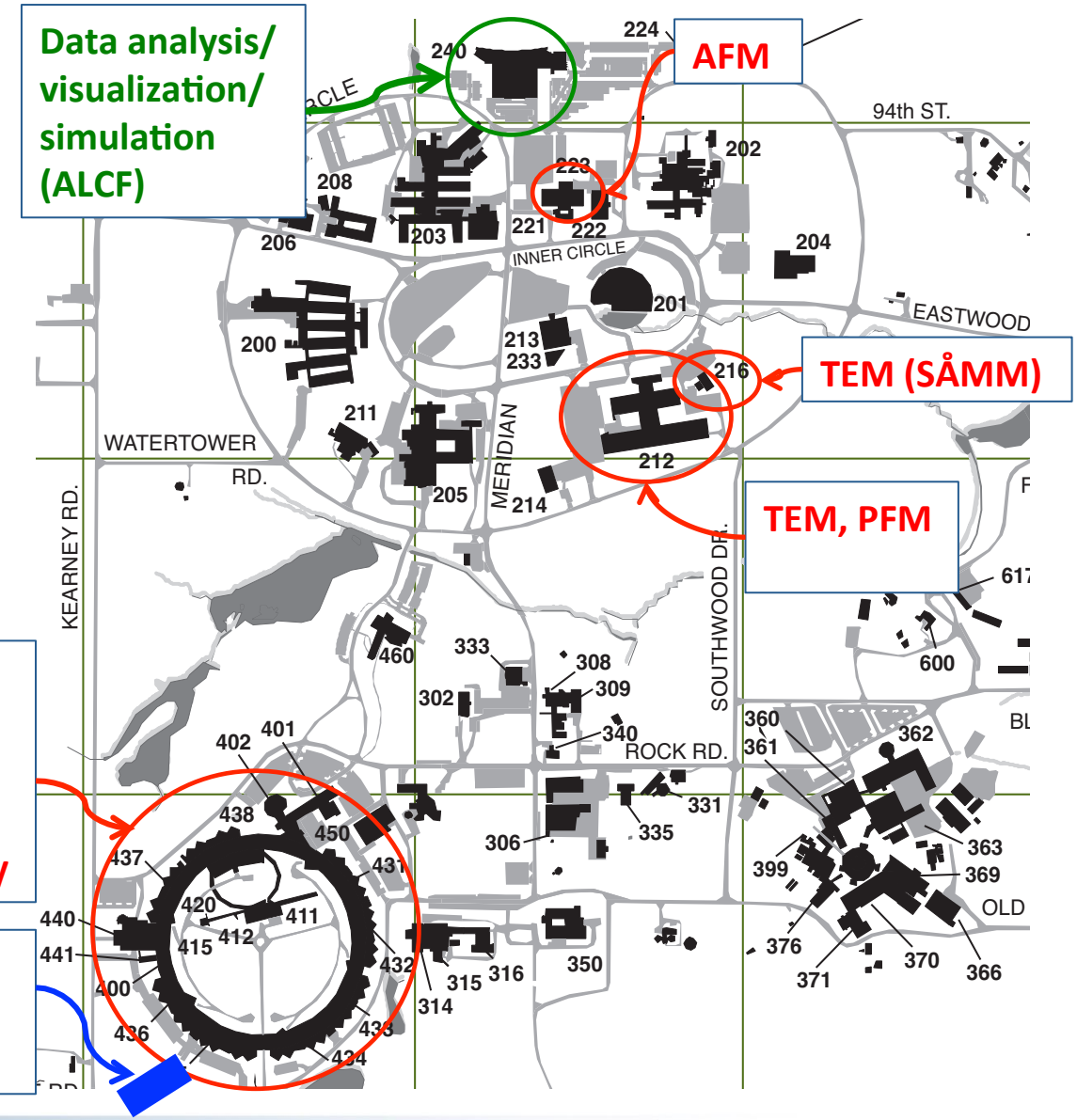




STEM tomography data shows the branched nature of the CFO filaments

Argonne's unique opportunity

… Integration!

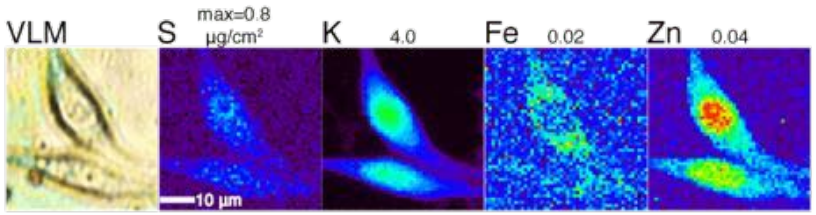


Integration

We are starting to benefit from collaborations and cross-connections, but imagine the strength and capabilities of an ***integrated approach at ANL***

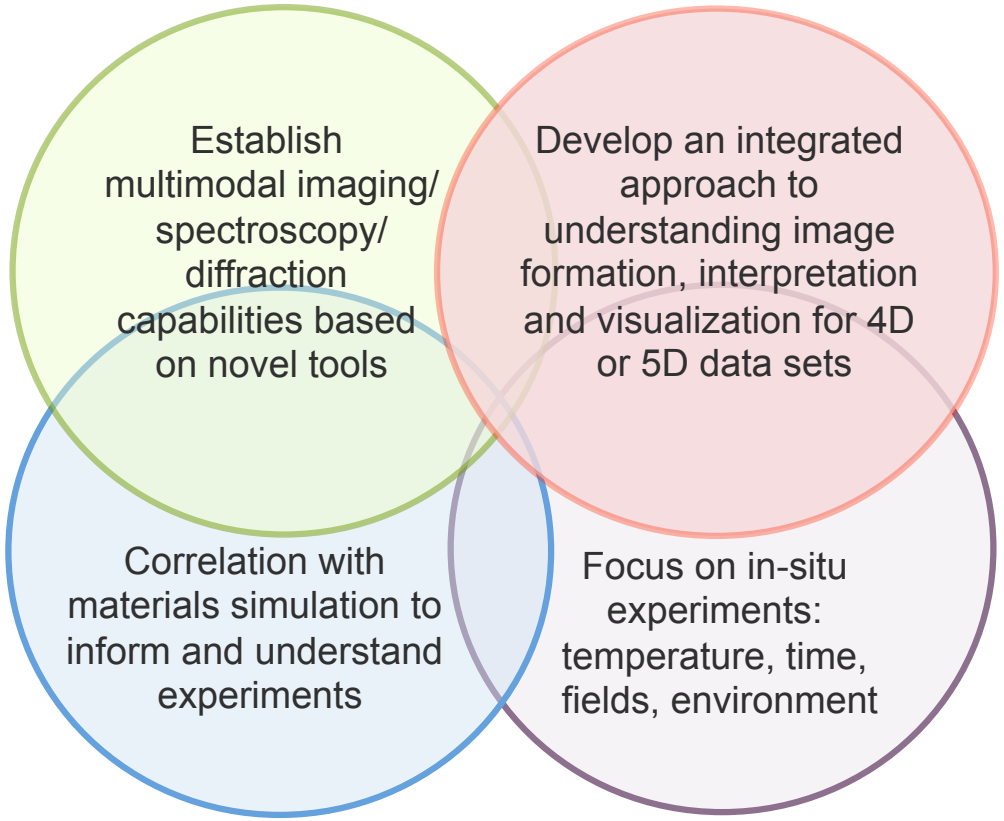
- Sample preparation facilities: common skills and instrumentation.
- Environmental chambers: common needs to provide pressure, fields, chemistry, temperature …
- Nanopositioning engineering expertise.
- "Big Data" extraction of scientific information from images.
- "Google Earth"-like views of multimode, multiscale data.
- Seamless integration between simulation, synthesis, and characterization.

- Energy Sciences Building
- Joint Center for Energy Storage Research
- Advanced Protein Crystallization Facility



Correlative cryo visible light microscopy (VLM) and x-ray fluorescence microscopy (elements S, K, Fe, Zn). Qiaoling Jin *et al.*

Argonne Integrated Imaging Initiative (I^3)



- **Close the loop** between design, synthesis and behavior
- **Integrate** ANL imaging capabilities
- **Portal** for external partners interested in engaging with Argonne in the imaging space

www.anl.gov/imaging

Argonne's User Facilities

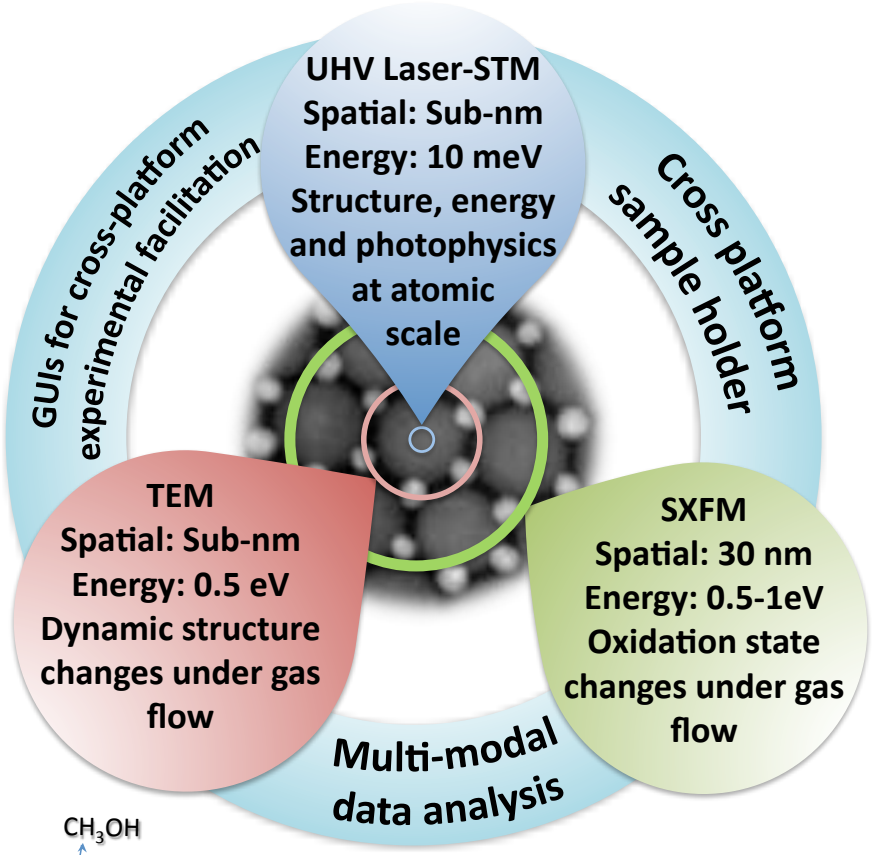
I^3 builds on and enhances the capabilities of Argonne's Scientific User Facilities

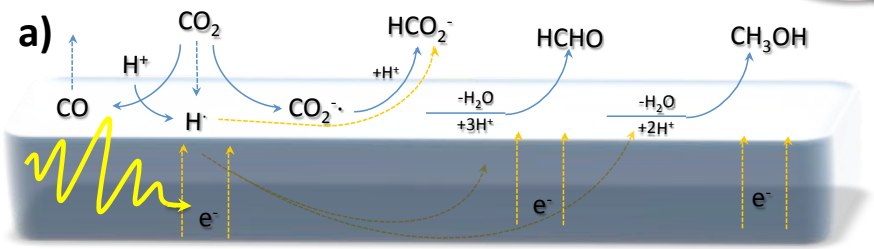
- Advanced Photon Source (APS): https://www1.aps.anl.gov/
- Center for Nanoscale Materials (CNM) including the Electron Microscopy Center: http://www.anl.gov/cnm/
- Argonne Leadership Computing Facility (ALCF): http://www.alcf.anl.gov/

I^3: First funded research programs

- Integrated Imaging to Understand and Advance Photocatalysis (PHOTO)
- Framework for Integrating Multimodal Imaging of Materials for Energy Storage (MIMES)
- Integrated Imaging, Modeling and Analysis of Ultrafast Energy Transport in Nanomaterials (MAUI)
- **Other talks from Argonne at this meeting:**
  - Monday, T6: D. Vine, "Real time phase retrieval in nanobeam ptychography"
  - Tuesday, T13: S. Sankaranarayanan, "Imaging and visualizing ultrafast energy transport via molecular simulations"
  - Wednesday, T30: D. Gürsoy, "Compressive sampling and its potentials in nanoimaging"
  - Wednesday, T31: F. De Carlo, "Data intensive science at synchrotron based 3D X-ray imaging facilities"

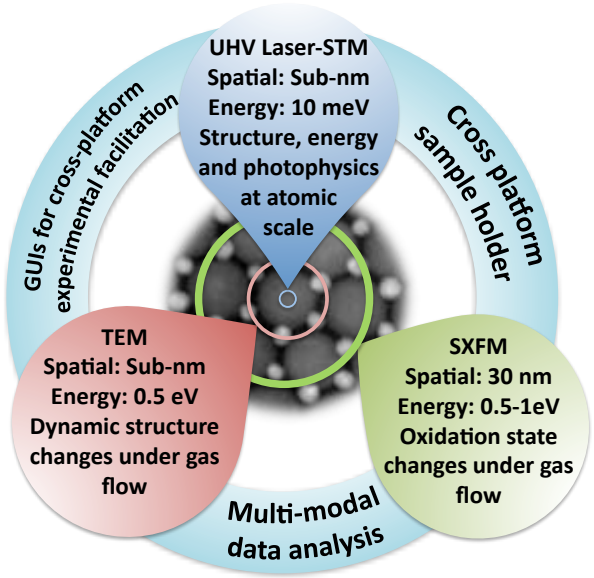
Integrated Imaging to Understand and Advance Photocatalysis (PHOTO): *J. Guest (NST) + NST, XSD, MSD*

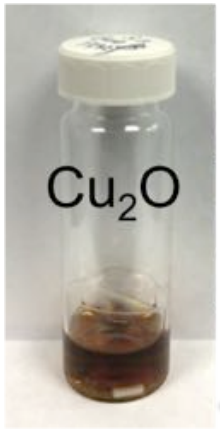




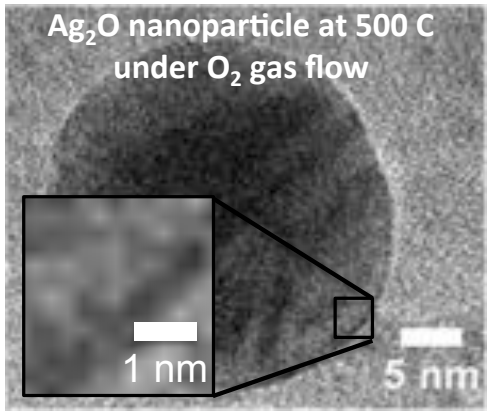
Integrated Imaging to Understand and Advance Photocatalysis (PHOTO): *J. Guest (NST) + NST, XSD, MSD*

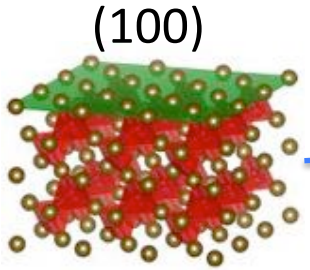
Goal:

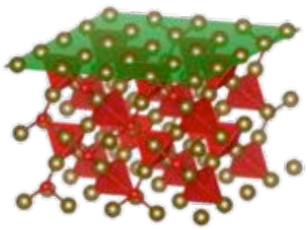




Gas-flow TEM

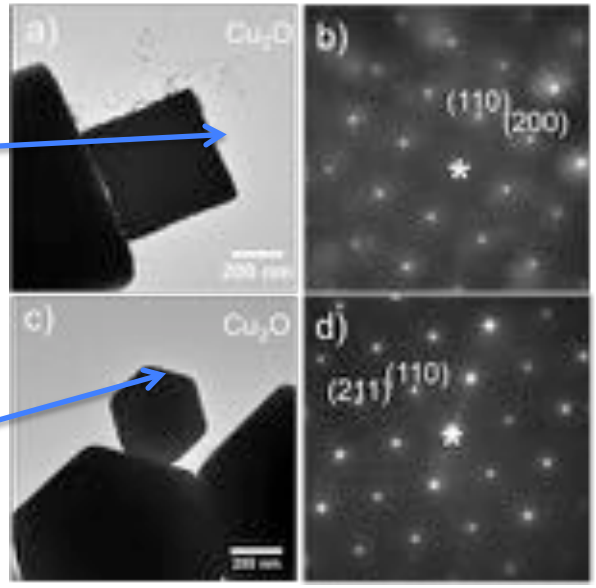






TEM images

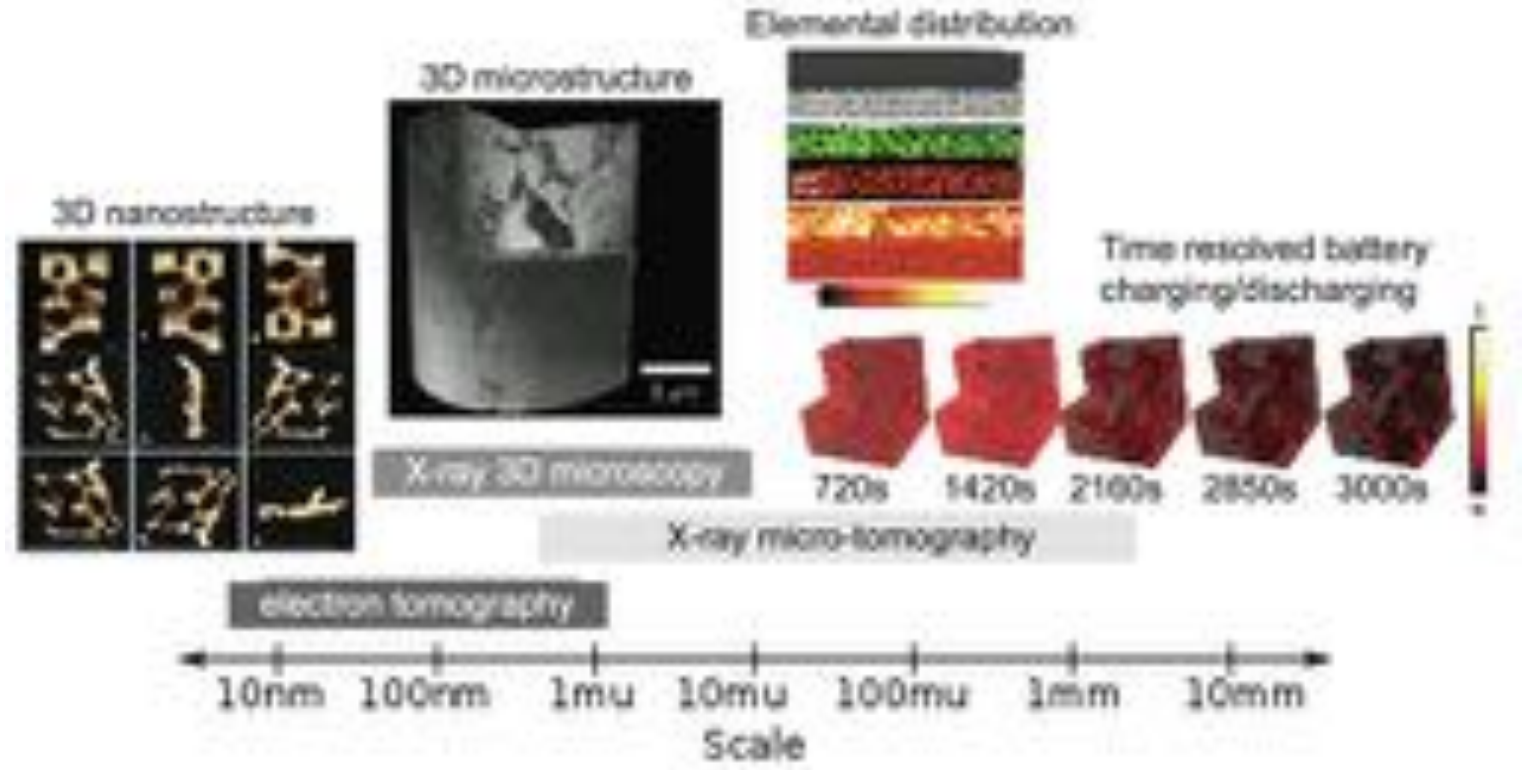
Selected area diffraction



FY15 Highlights

- Cross-platform (TEM, x-ray) sample holder with gas-flow and optical access under development and testing
- Cu_2O nanoparticles with different crystal facets were successfully synthesized to explore relative photo-catalytic reduction of CO_2

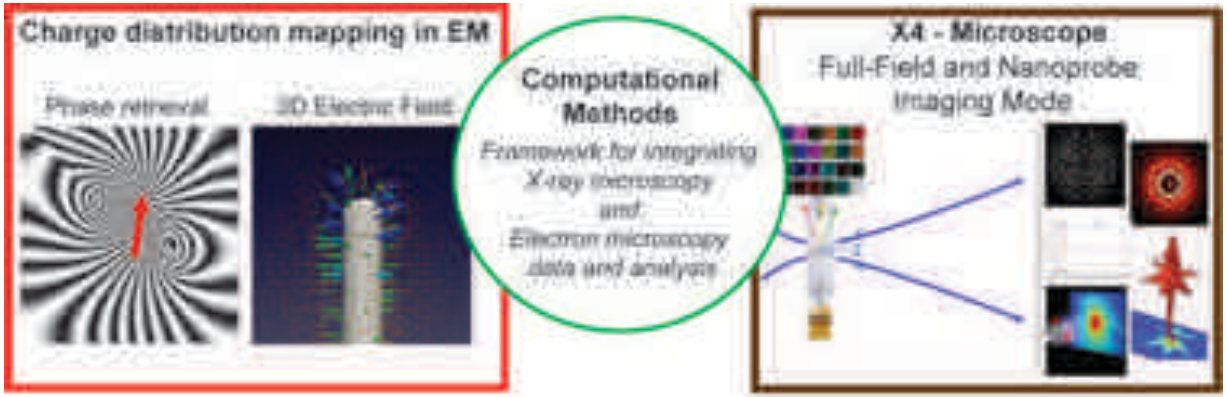
Framework for Integrating Multimodal Imaging of Materials for Energy Storage (MIMES): *D. Gürsoy (XSD) + MSD, CSE, NU*



Opportunity: Correlate 3D x-ray and electron data from batteries to understand structure and aging processes over wide range of length scales, and to develop a computational framework for multimodal imaging of these structures and materials.

Framework for Integrating Multimodal Imaging of Materials for Energy Storage (MIMES): *D. Gürsoy (XSD) + MSD, CSE, NU*

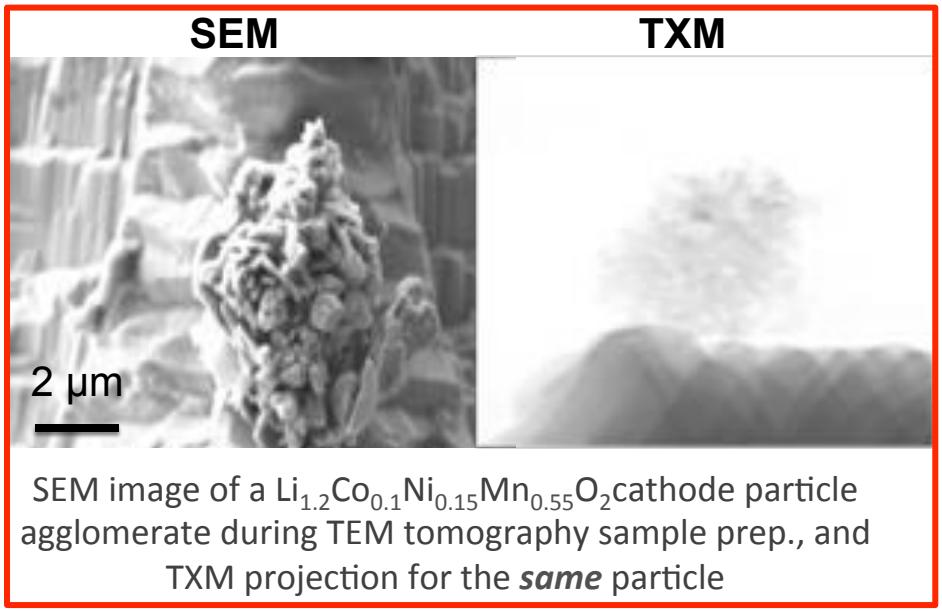
Goal:



FY15 Highlights

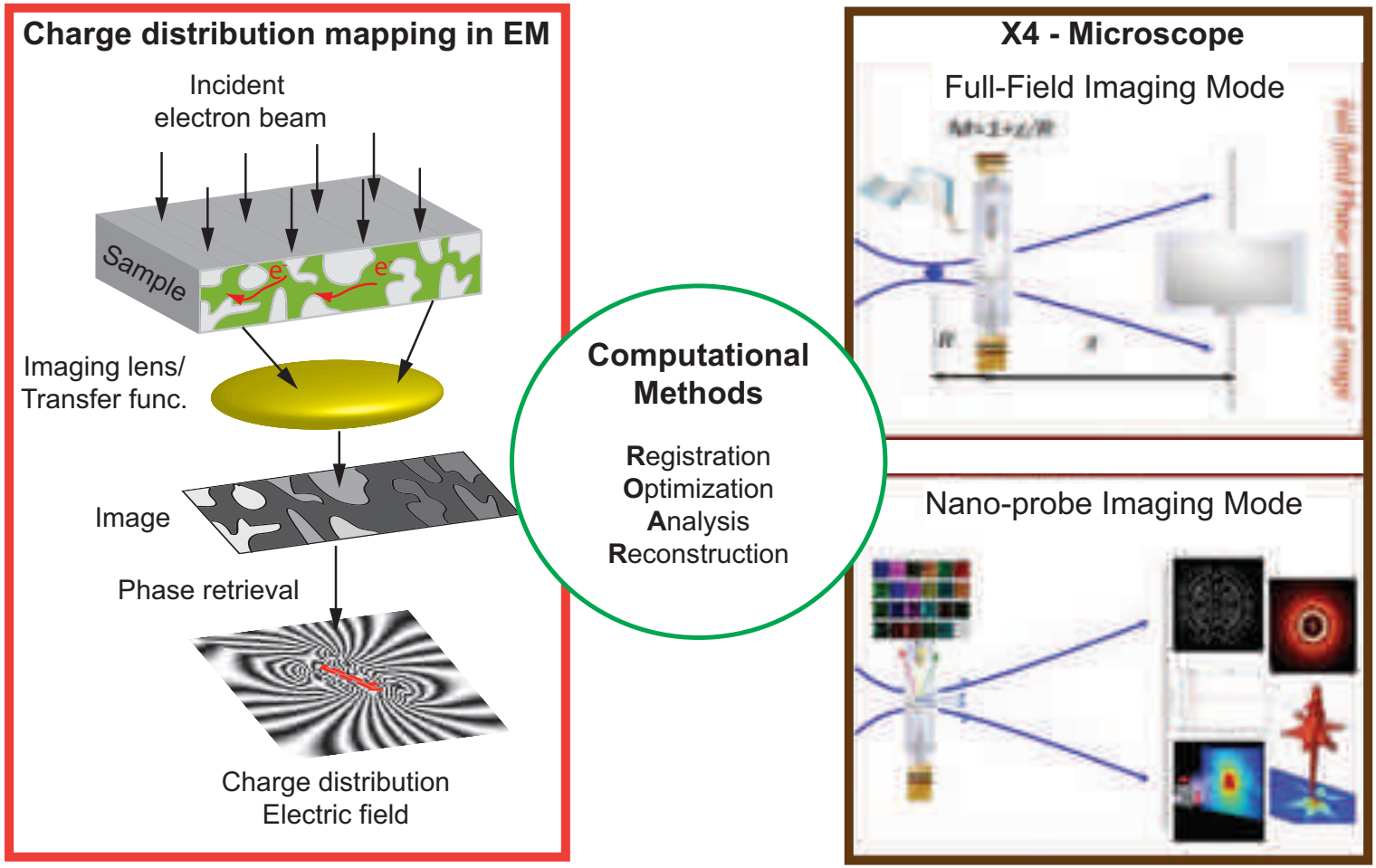
- 3D electron microscopy data analysis integrated into tomography software
- Improved tomographic reconstruction methods for electron microscopy [1]
- Initial experiments integrating X-ray and electron tomography of the same region

C. Phatak, Ultramicroscopy 150, 54 (2015)



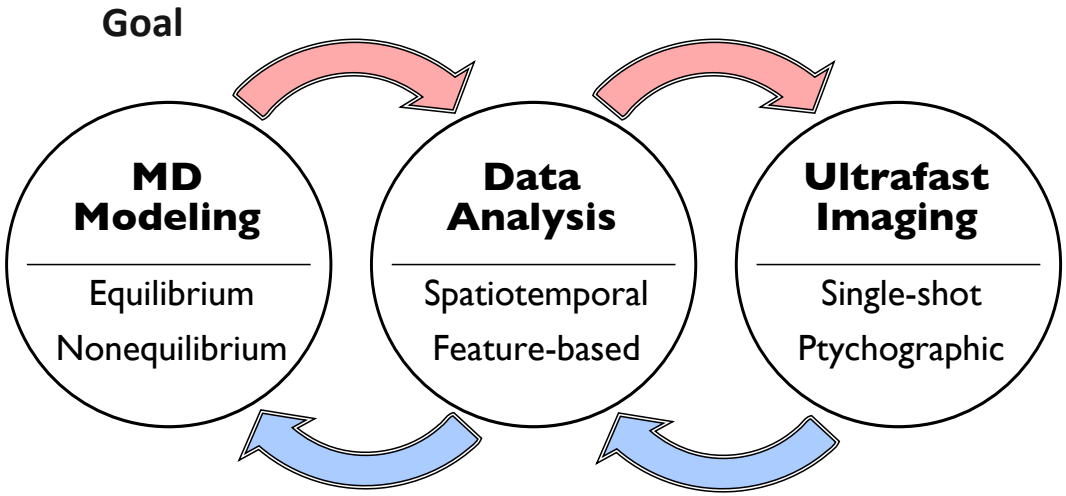
SEM image of a $Li_{1.2}Co_{0.1}Ni_{0.15}Mn_{0.55}O_2$ cathode particle agglomerate during TEM tomography sample prep., and TXM projection for the ***same*** particle

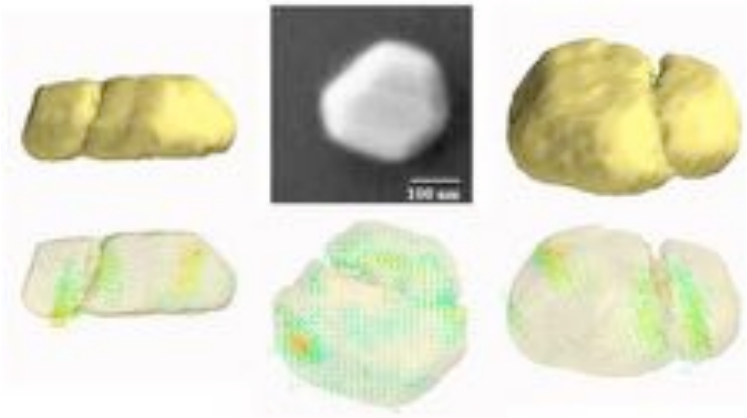
Framework for Integrating Multimodal Imaging of Materials for Energy Storage (MIMES): *D. Gürsoy (XSD) + MSD, CSE, NU*

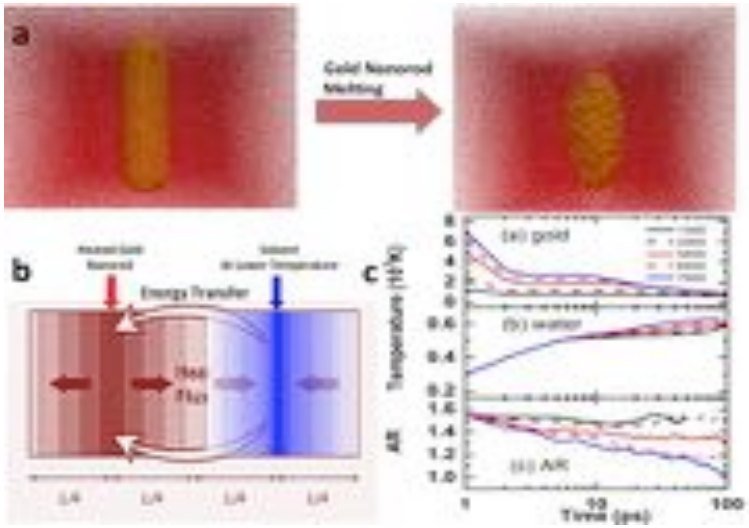


- Using Globus Online to transport data

Integrated Imaging, Modeling and Analysis of Ultrafast Energy Transport in Nanomaterials (MAUI): *T. Peterka(MCS) + MCS,XSD,NST*





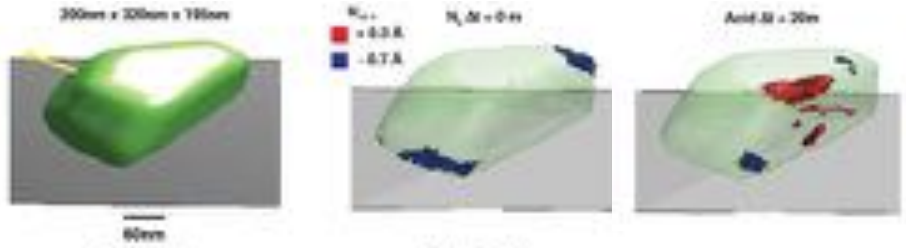


Integrated Imaging, Modeling and Analysis of Ultrafast Energy Transport in Nanomaterials (MAUI): *T. Peterka(MCS) + MCS,XSD,NST*

FY15 Highlight

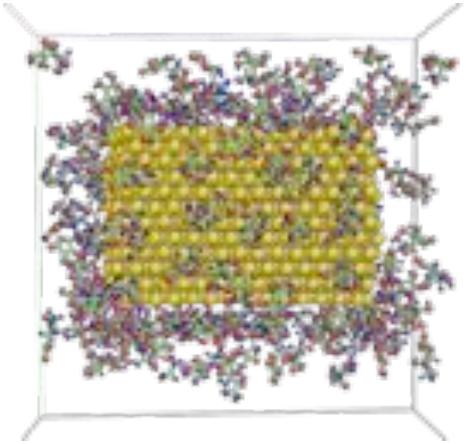
- Reactive MD simulation of decomposition of ascorbic acid on Au nanoparticle is enabling understanding of experimental 3D X-ray data obtained by MAUI PI prior to the LDRD project

Au nanoparticle in ascorbic acid imaged using coherent x-rays (Harder, XSD and Ulvestad, UCSD)

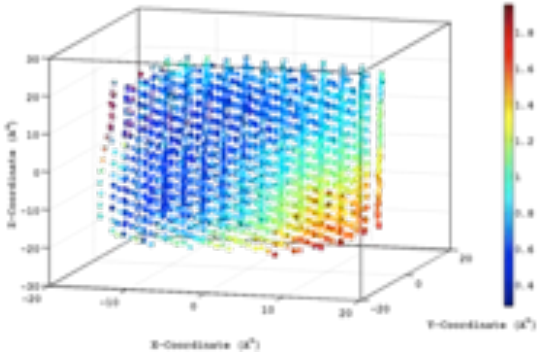


- Lattice displacement at corners of flattest facet
- Electron injection create largest electric field at these sites: "hot spots" for the reaction

Sankaranarayanan and Deshmukh (ANL/NST)



Ascorbic acid adsorbs at a low coordinated corner site. Subsequent dissociation leads to ~40% strain



Relative displacement of Au atoms compared to initial lattice

I^3 Workshop on Tomography and Ptychography, Sept 29-30, 2014

- 23 invited talks and ~20 posters
  - 9 speakers were external to Argonne, including one international speaker

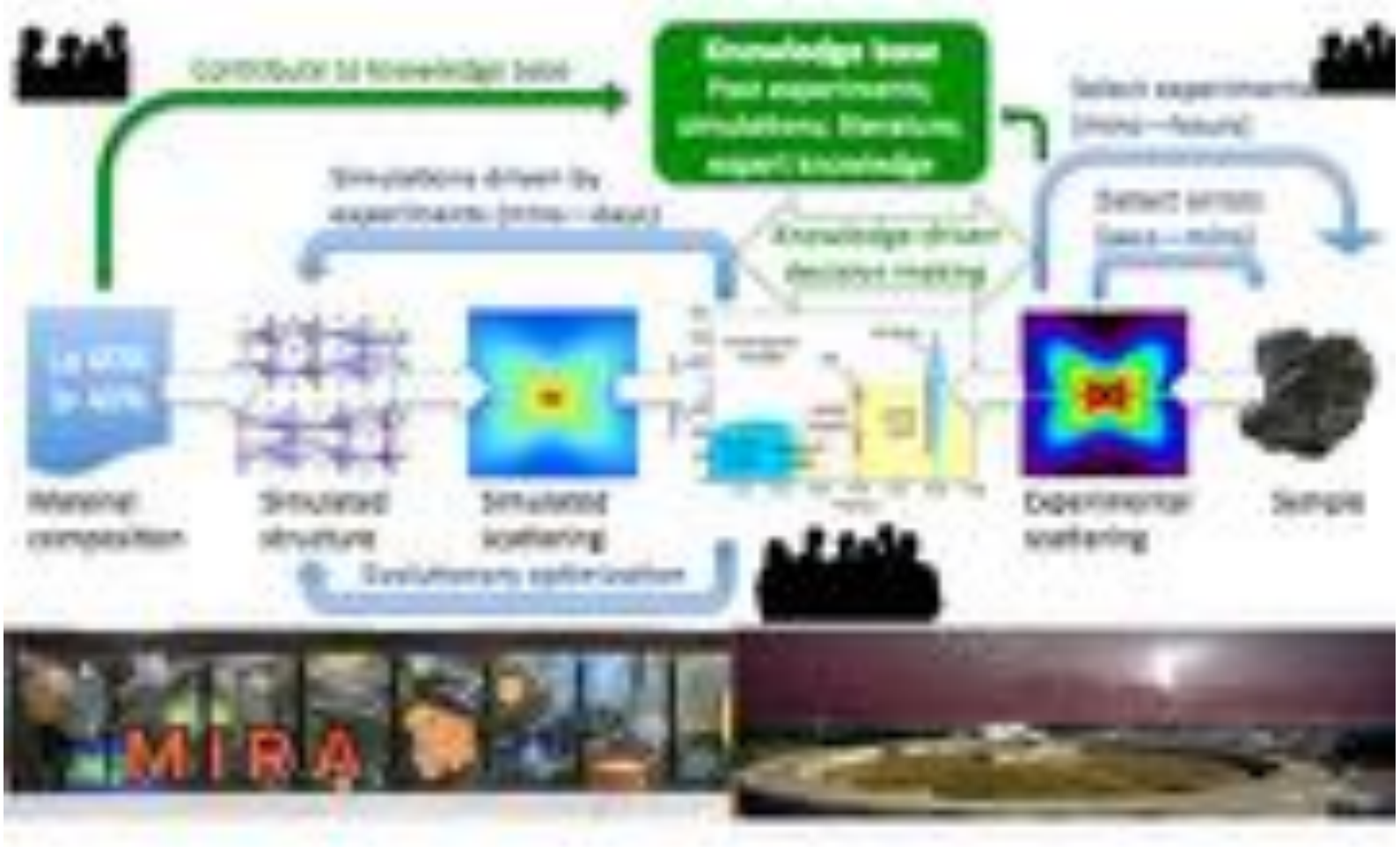
- Brought together 92 attendees with interest in experimental imaging, image and data analysis and visualization

- Biweekly seminars: initially internal, now have funds to invite external speakers

Integrated Imaging at ANL in addition to I^3

- See highlights at **www.anl.gov/imaging**

Argonne Grand Challenge on “Data Driven Science”



See F. De Carlo's talk on Big Data this Wednesday

Summary

- The ***Argonne Integrated Imaging Initiative*** provides an interdisciplinary bridge across Argonne's imaging capabilities and communities
- Argonne is actively developing three key I^3 directions and funding them through a strategic LDRD initiative
- We are engaging local universities (Purdue, NU, UC, UIC …) and industries (AMBER, Hummingbird, Seagate, …)
- We are leveraging DOE ASCR and BES as well as Argonne LDRD funded projects across the lab
- Argonne is planning to upgrade ALCF and APS – **we have both under the same roof!**

www.anl.gov/imaging

Acknowledgments

Amanda Petford-Long	Argonne I^3 Initiative Lead ANL/MSD, Northwestern
Chris Jacobsen	X-ray Science Division ANL/APS, Northwestern
Francesco De Carlo	X-ray Imaging Group ANL/APS
Doga Gürsoy	X-ray Imaging Group ANL/APS
Tom Peterka	Data-Intensive Science Group ANL/MCS
Jeff Guest	CNM EMMD Group ANL/NST
Dean Miller	CNM Electron Microscopy Center ANL/NST

and Thank You !