A Multimodal Approach:
How to Apply Synchrotron X-ray Characterization and Beyond to Tackle YOUR Research Challenges?

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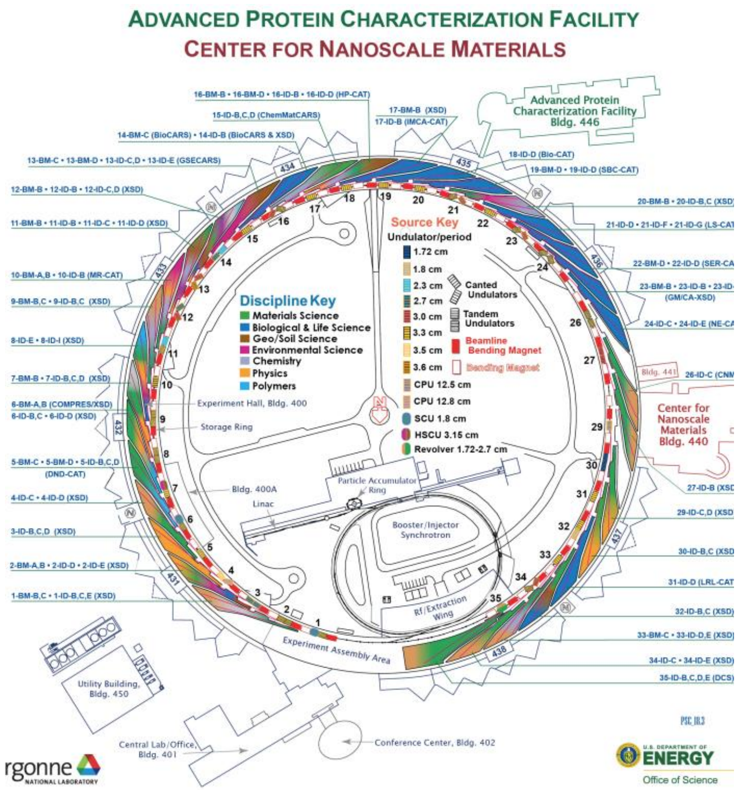
26th National School on Neutron and X-ray Scattering
Friday, August 2nd, Multi-Modal Experiments

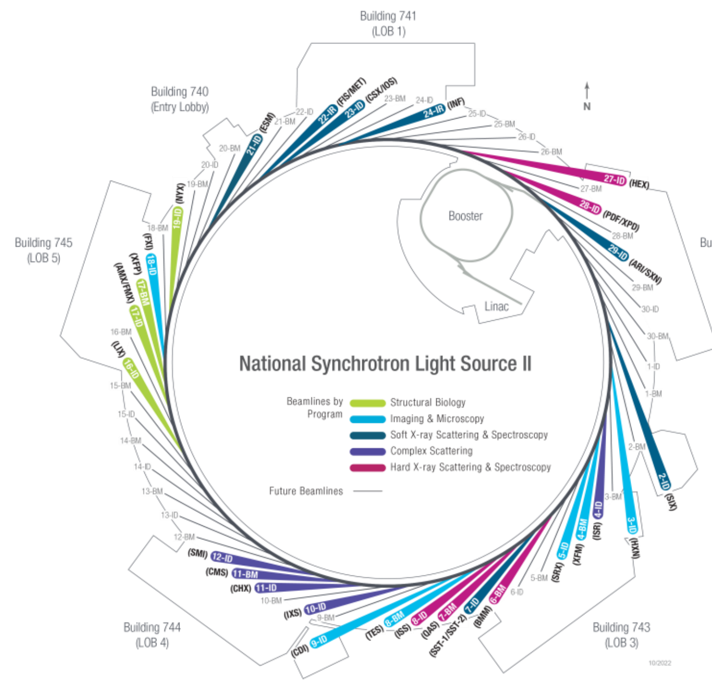
A suite of cutting-edge characterization tools!

Advanced Photon Source (APS)



https://www.aps.anl.gov/Beamlines/Beamlines-Map

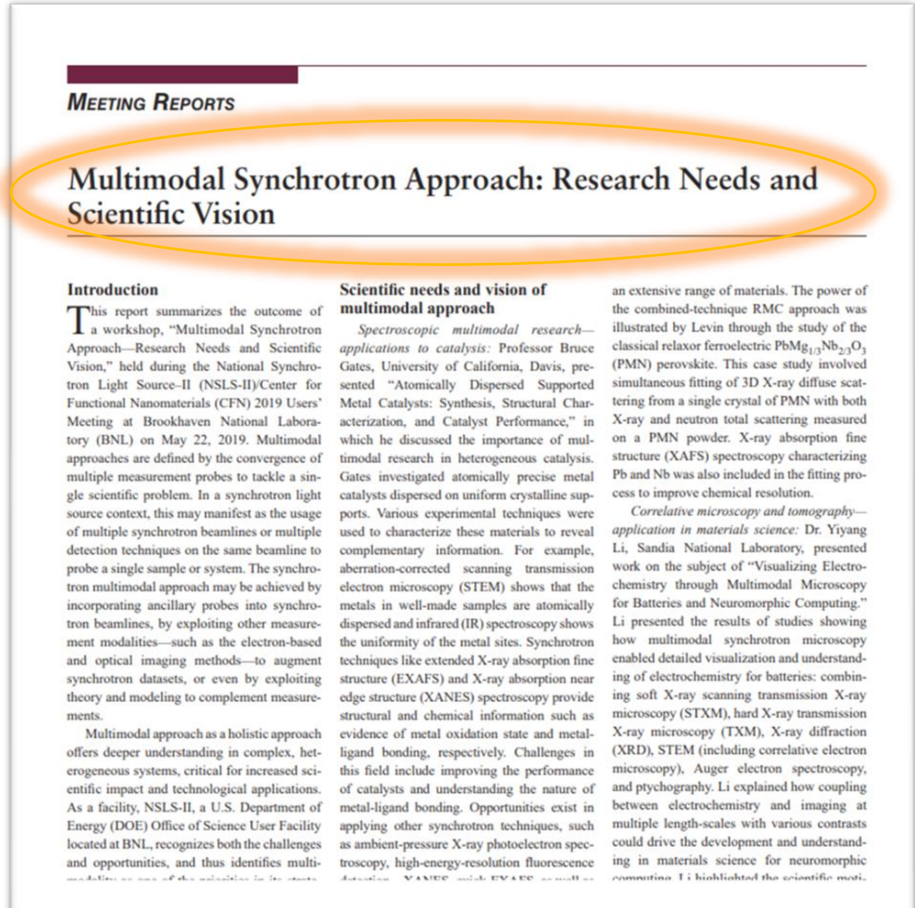
National Synchrotron Light Source II (NSLS-II)



https://www.bnl.gov/nsls2/beamlines/map.php

A good reference: 2020 Workshop Report

- **"Multimodal Synchrotron Approach: Research Needs and Scientific Vision"**
  Yu-Chen Karen Chen-Wiegart, Iradwikanari Waluyo, Andrew Kiss, Stuart Campbell, Lin Yang, Eric Dooryhee, Jason R. Trelewicz, Yiyang Li, Bruce Gates, Mark Rivers, Kevin G. Yager
  Synchrotron Radiation News (2020)
  DOI: 10.1080/08940886.2020.1701380



MEETING REPORTS

Multimodal Synchrotron Approach: Research Needs and Scientific Vision

Introduction

This report summarizes the outcome of a workshop, "Multimodal Synchrotron Approach—Research Needs and Scientific Vision," held during the National Synchrotron Light Source–II (NSLS-II)/Center for Functional Nanomaterials (CFN) 2019 Users' Meeting at Brookhaven National Laboratory (BNL) on May 22, 2019. Multimodal approaches are defined by the convergence of multiple measurement probes to tackle a single scientific problem. In a synchrotron light source context, this may manifest as the usage of multiple synchrotron beamlines or multiple detection techniques on the same beamline to probe a single sample or system. The synchrotron multimodal approach may be achieved by incorporating ancillary probes into synchrotron beamlines, by exploiting other measurement modalities—such as the electron-based and optical imaging methods—to augment synchrotron datasets, or even by exploiting theory and modeling to complement measurements.

Multimodal approach as a holistic approach offers deeper understanding in complex, heterogeneous systems, critical for increased scientific impact and technological applications. As a facility, NSLS-II, a U.S. Department of Energy (DOE) Office of Science User Facility located at BNL, recognizes both the challenges and opportunities, and thus identifies multi-

Scientific needs and vision of multimodal approach

Spectroscopic multimodal research—applications to catalysis: Professor Bruce Gates, University of California, Davis, presented "Atomically Dispersed Supported Metal Catalysts: Synthesis, Structural Characterization, and Catalyst Performance," in which he discussed the importance of multimodal research in heterogeneous catalysis. Gates investigated atomically precise metal catalysts dispersed on uniform crystalline supports. Various experimental techniques were used to characterize these materials to reveal complementary information. For example, aberration-corrected scanning transmission electron microscopy (STEM) shows that the metals in well-made samples are atomically dispersed and infrared (IR) spectroscopy shows the uniformity of the metal sites. Synchrotron techniques like extended X-ray absorption fine structure (EXAFS) and X-ray absorption near edge structure (XANES) spectroscopy provide structural and chemical information such as evidence of metal oxidation state and metal-ligand bonding, respectively. Challenges in this field include improving the performance of catalysts and understanding the nature of metal-ligand bonding. Opportunities exist in applying other synchrotron techniques, such as ambient-pressure X-ray photoelectron spectroscopy, high-energy-resolution fluorescence

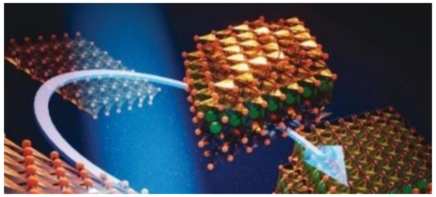
an extensive range of materials. The power of the combined-technique RMC approach was illustrated by Levin through the study of the classical relaxor ferroelectric $PbMg_{1/3}Nb_{2/3}O_3$ (PMN) perovskite. This case study involved simultaneous fitting of 3D X-ray diffuse scattering from a single crystal of PMN with both X-ray and neutron total scattering measured on a PMN powder. X-ray absorption fine structure (XAFS) spectroscopy characterizing Pb and Nb was also included in the fitting process to improve chemical resolution.

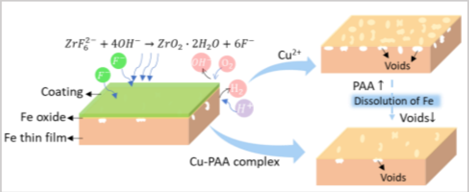
Correlative microscopy and tomography—application in materials science: Dr. Yiyang Li, Sandia National Laboratory, presented work on the subject of "Visualizing Electrochemistry through Multimodal Microscopy for Batteries and Neuromorphic Computing." Li presented the results of studies showing how multimodal synchrotron microscopy enabled detailed visualization and understanding of electrochemistry for batteries: combining soft X-ray scanning transmission X-ray microscopy (STXM), hard X-ray transmission X-ray microscopy (TXM), X-ray diffraction (XRD), STEM (including correlative electron microscopy), Auger electron spectroscopy, and ptychography. Li explained how coupling between electrochemistry and imaging at multiple length-scales with various contrasts could drive the development and understanding in materials science for neuromorphic

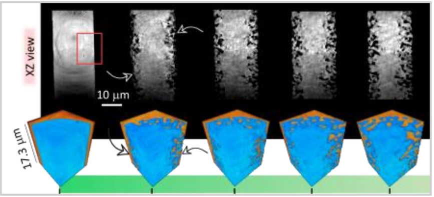
Our Research Program on Functional Materials with Synchrotron X-ray Analysis

1) Materials by Design:
Nano-Architectured Porous Metals and Metallic Composites

2) Sustainable Energy:
Multimodal Synchrotron Studies of Energy Storage







4) Sustainable Manufacturing:
Environmentally friendly functional coating

3) Sustainable Energy:
Interfacial Processes of Materials in Molten Salts and Extreme Environments

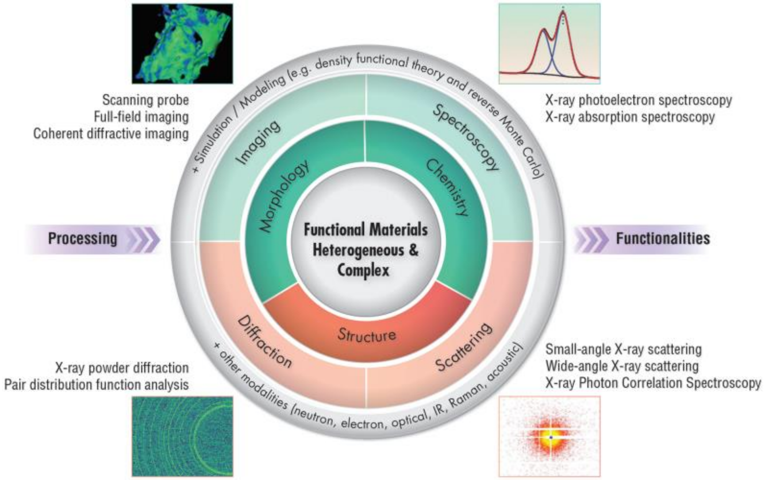
WIIFM?
What's in it for me?

- What is a multimodal approach?
- Why we care about it?

- *Research example: Conversion coating*

- Ways to frame multimodal analysis.

- *Research example: Battery*



- Beyond synchrotron
  - Other experimental modalities
  - Experiment – simulation feedback loop
  - Data science opportunities

- *Research example: Molten Salt and Dealloying*

2-Min You Talk!

Talk to your neighbor(s):

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2) What are the **main techniques (2-5 of them)** you use to characterize them? (Name at least one X-ray or neutron technique, if possible!)

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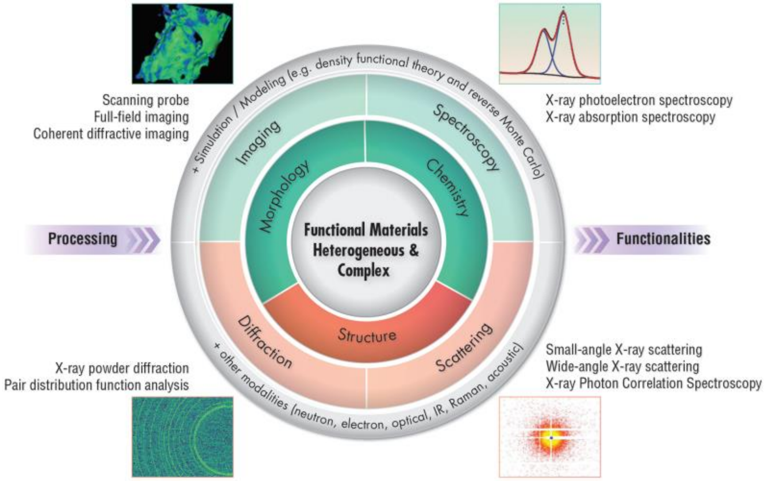
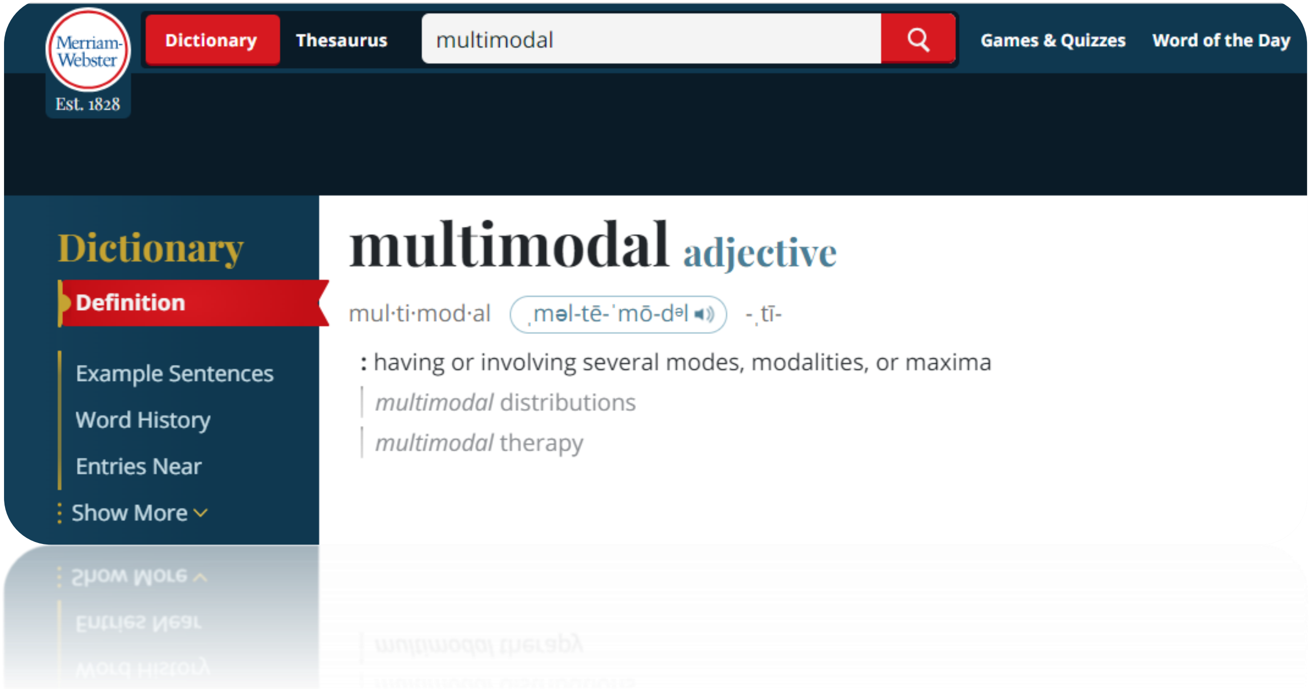


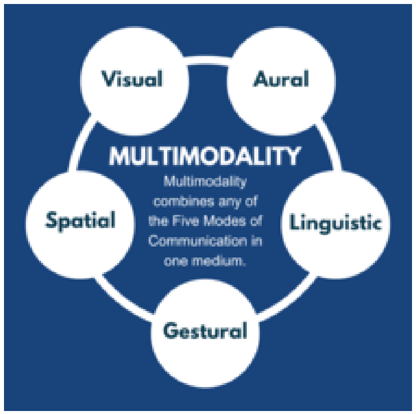
What is multimodal?

- Dictionary definition:
  - https://www.merriam-webster.com/dictionary/multimodal

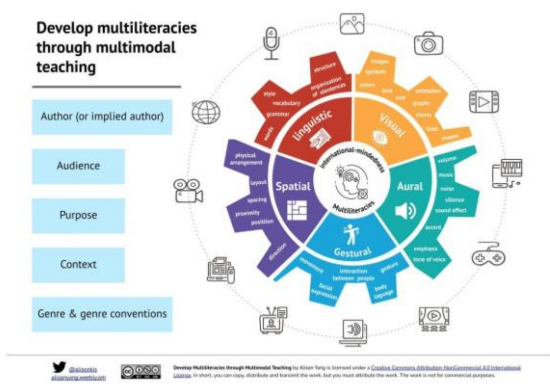


Multimodality everywhere!

Multimodal Pedagogy/Teaching

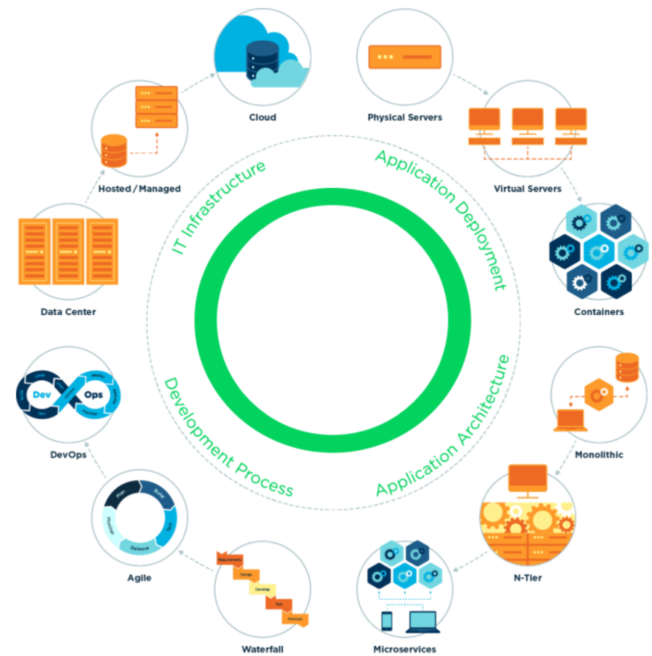


https://en.wikipedia.org/wiki/Multimodal_pedagogy



https://alisonyang.com/multimodal-teaching/

Multimodal IT



https://www.suse.com/c/the-rise-of-multimodal-it-and-what-it-means-to-you/

Multimodal Customer Experience

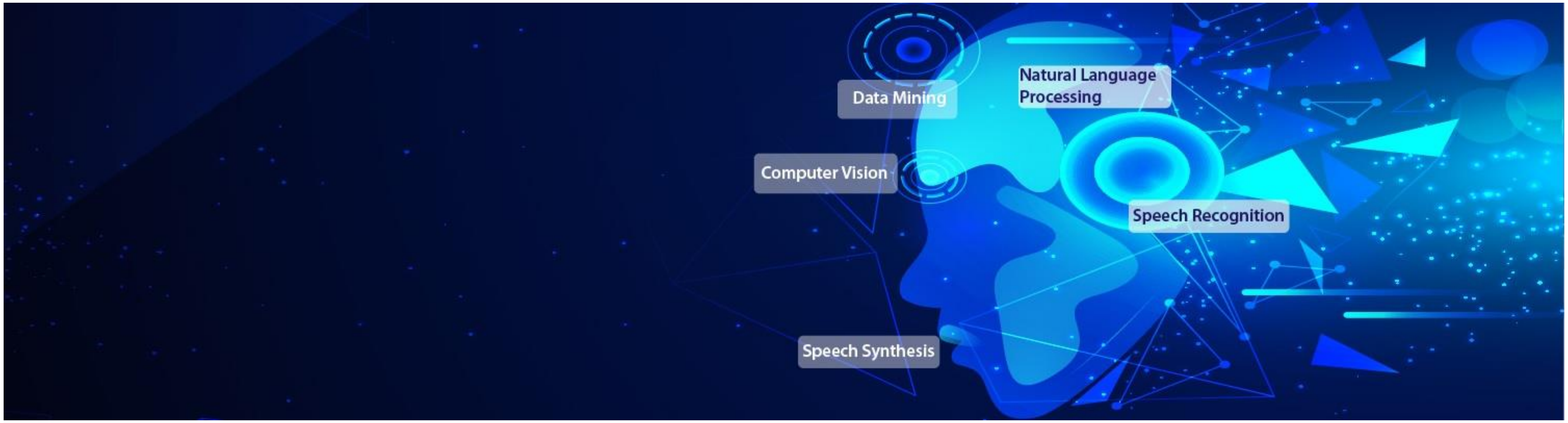
https://www.uniphore.com/blog/what-s-a-multimodal-customer-experience/

Multimodal Transport

Multimodal transport, also known as combined transport, is a transport system that involves the movement of goods using multiple modes of transport such as trucks, rail, air and ships.

https://www.morethanshipping.com/what-is-multimodal-transport/

Multimodal Artificial Intelligence!



https://www.aimesoft.com/multimodalai.html

Multimodal AI is a new AI paradigm, in which various data types (image, text, speech, numerical data) are combined with multiple intelligence processing algorithms to achieve higher performances. Multimodal AI often outperforms single modal AI in many real-world problems.

Ecosystem!!

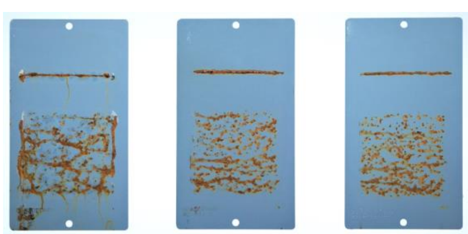
What is the ecosystem of synchrotron (and neutron) characterization?

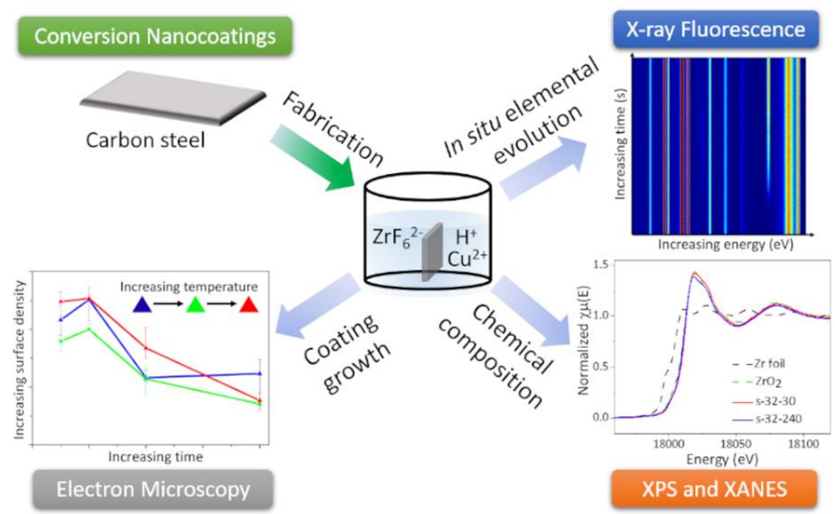
Multimodality – In the context of scientific research

- *"Multimodal approaches are defined by the convergence of multiple measurement probes to tackle a single scientific problem."*

Karen Chen-Wiegart et al., Synchrotron Radiation News (2020)

We have already been applying multimodal characterization from the beginning!





Xiaoyang Liu, ACS Applied Nanomaterials, 2019

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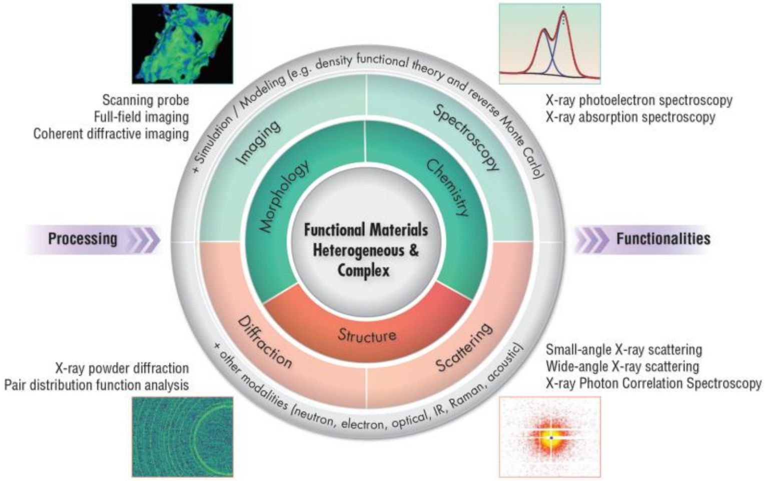


Why taking a multimodal approach?

Synchrotron offers a suite of the amazing characterization tools!!

Awesome playground!!
Lots of opportunities!!
Unprecedent information!!

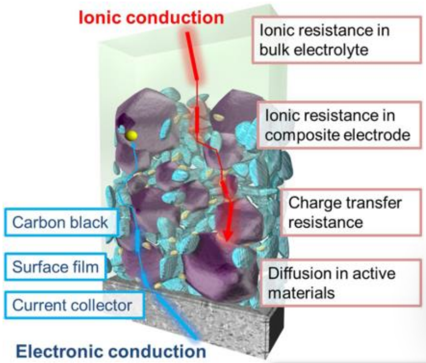
Easily get lost
– why am I doing what I am doing?

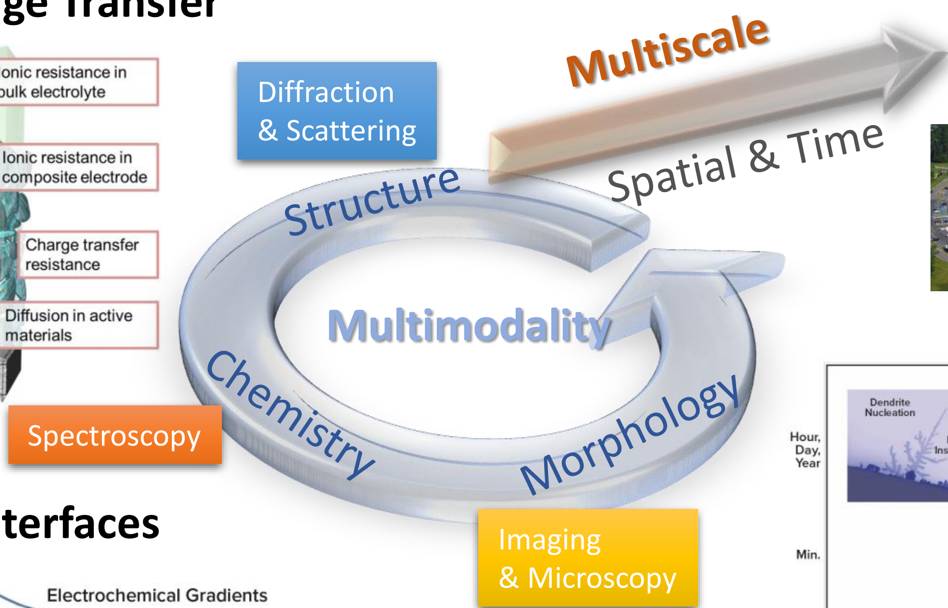
- *Multimodal approach as a holistic approach offers deeper understanding in **complex, heterogeneous systems**, critical for increased scientific impact and technological applications.*

Karen Chen-Wiegart et al., Synchrotron Radiation News (2020)

Research challenges complex, heterogeneous systems

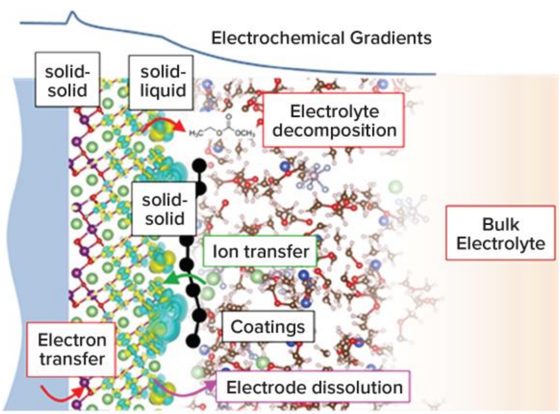
Mass and Charge Transfer

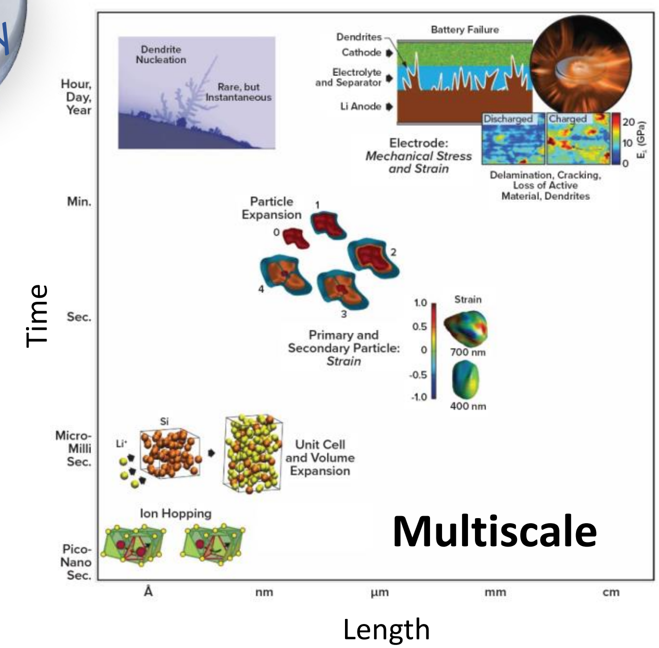




Multimodal Synchrotron X-ray Characterization

Bulk and Interfaces





2-Min You Talk!

Talk to your neighbor(s):

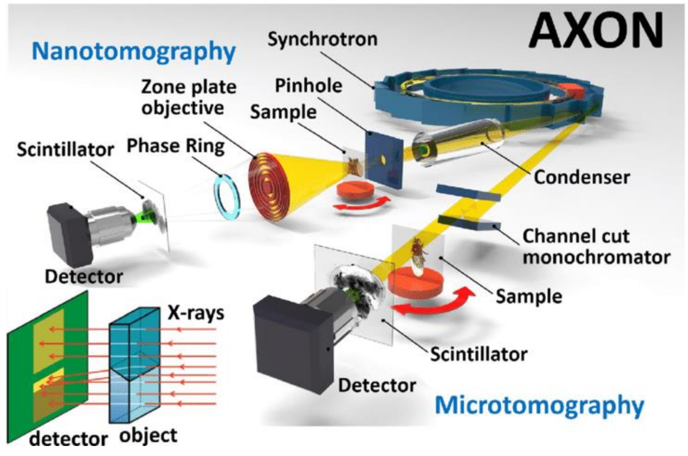
1) What is your research topic? (An "elevator pitch")
2) What are the main techniques (2-5 of them) you use to characterize them? (Name at least one X-ray or neutron technique, if possible!)
3) **Why are you using them?**
   What information can you get out of each of the techniques?
   Are they complementary to each other?

Multimodal Synchrotron Approach

- In a synchrotron light source context, this may manifest as the usage of

1) **Multiple synchrotron beamlines** or
2) **Multiple detection techniques on the same beamline**

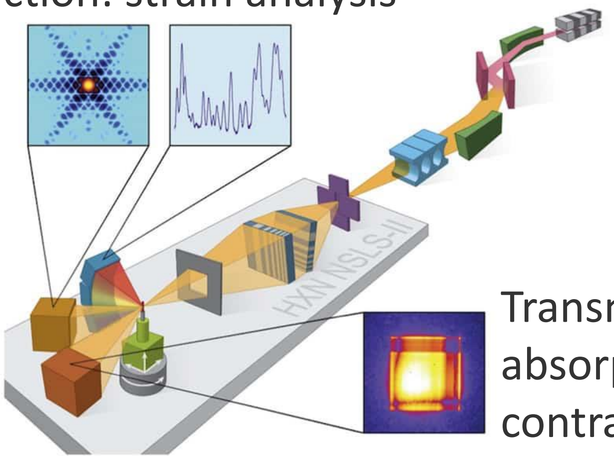
to probe a single sample or system.



Hwu, Y et al., BMC Biol 15, 122 (2017). https://doi.org/10.1186/s12915-017-0461-8

Fluorescence: elemental mapping

Diffraction: strain analysis



Transmission: absorption/phase-contrast imaging

Hanfei Yan et al., 2018 Nano Futures 2 011001 DOI 10.1088/2399-1984/aab25d

Why using different beamlines?

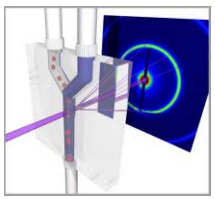
Suite of beamlines with complementary techniques - enabling time-resolved, *operando*, multi-modal and multi-dimensional studies

Scattering | **Diffraction** | **Spectroscopy** | **Imaging**

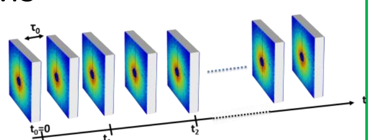
Structure

Chemistry

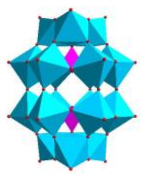
Morphology



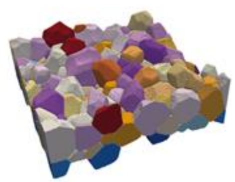
CMS



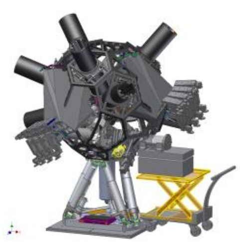
CHX

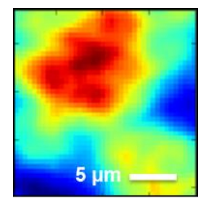


XPD



ISS

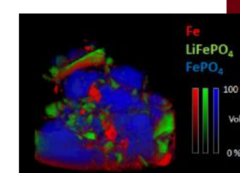




SRX

HXN

FXI



(XPD): X-ray Powder Diffraction

(ISS): Inner Shell Spectroscopy

(SRX): Sub-micron Resolution X-ray Spectroscopy

(CMS): Complex Materials Scattering

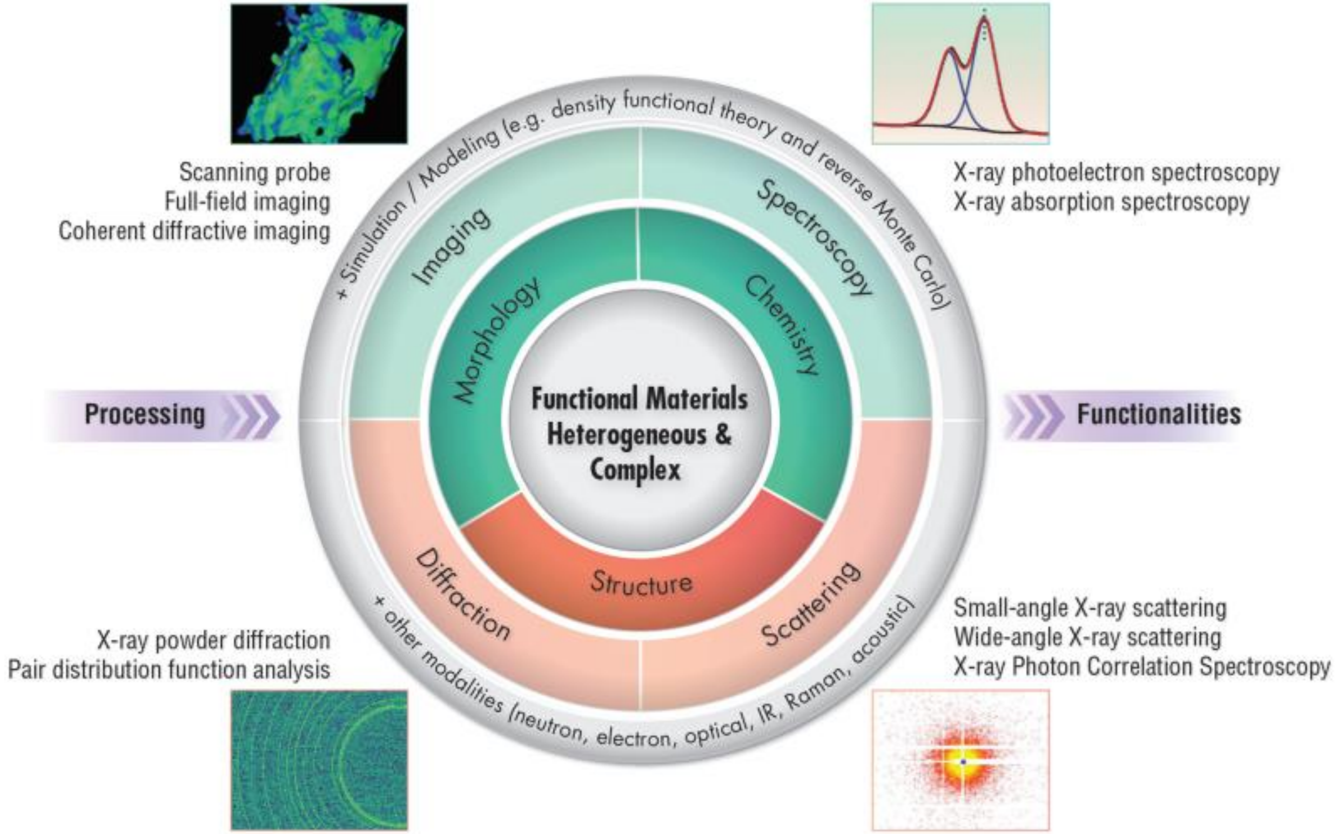
(HXN): Hard X-ray Nanoprobe

(CHX): Coherent Hard X-ray: XPCS

(FXI): Full-Field X-ray Imaging

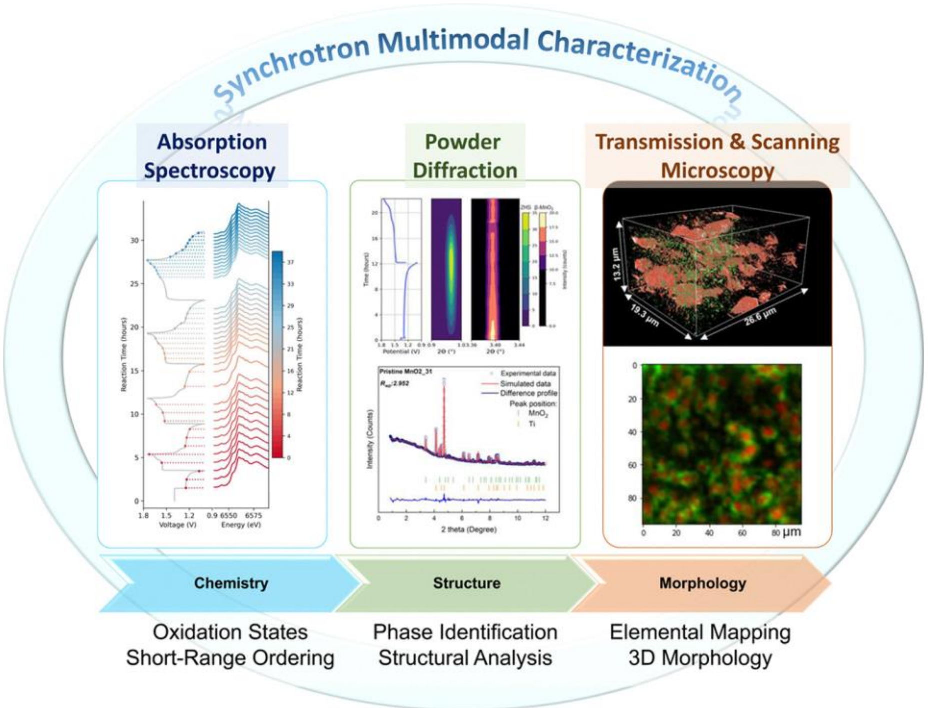
1. What is the processing – structure – property relationship?
(How do we control the properties?)

2. How do the materials' morphology, chemistry and structure evolve as a function of time and processing/operating conditions?



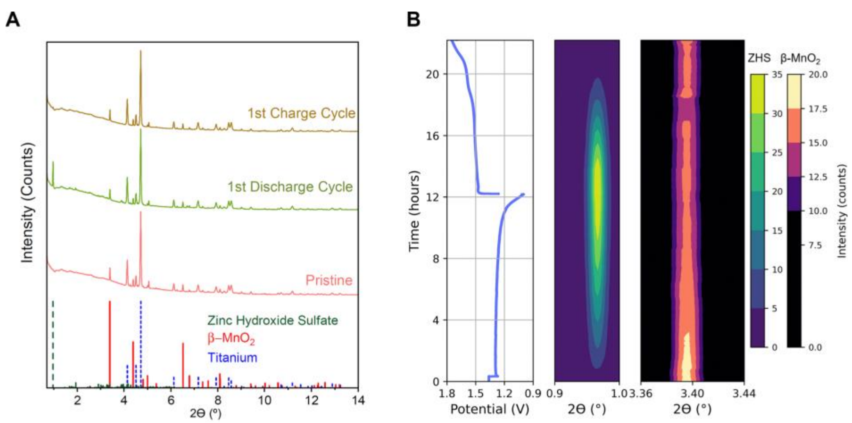
Karen Chen-Wiegart et al., Synchrotron Radiation News (2020)

Towards better understanding of reaction mechanism by *operando* multi-modal X-ray synchrotron characterization



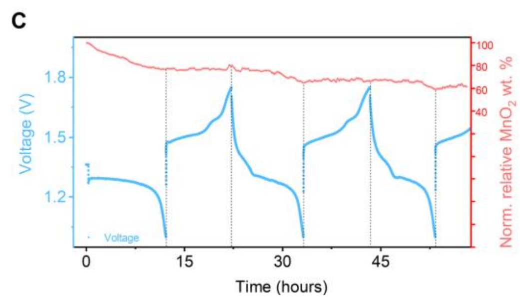
- *Varun R. Kankanallu, Xiaoyin Zheng, Denis Leschev, Nicole Zmich, Charles Clark, Cheng-Hung Lin, Hui Zhong, Sanjit Ghose, Andrew M. Kiss, Dmytro Nykypanchuk, Eli Stavitski, Esther S. Takeuchi, Amy C. Marschilok, Kenneth J. Takeuchi, Jianming Bai, Mingyuan Ge* and Yu-chen Karen Chen-Wiegart, Energy & Environmental Science (2023), DOI: 10.1039/D2EE03731A*

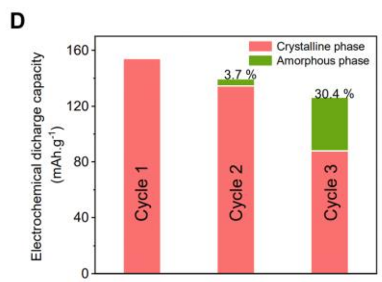
Operando X-ray diffraction: Phase evolution



- Phase evolution of the β-MnO_2 electrode at the pristine, half-cycle and full-cycle states.
- The galvanostatic discharge–charge profile for the first cycle and its corresponding waterfall plot indicate the formation and disappearance of the zinc hydroxy sulfate (ZHS) phase and gradual reduction in MnO_2 peak intensity.

- Normalized relative MnO_2 weight percentage vs. the electrochemical potential for the first ~ 3 cycles.
- Relative capacity contribution by the amorphous phase in the 2nd and 3rd cycles.





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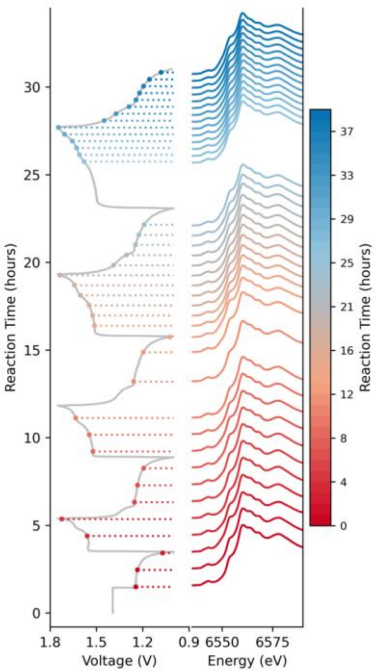
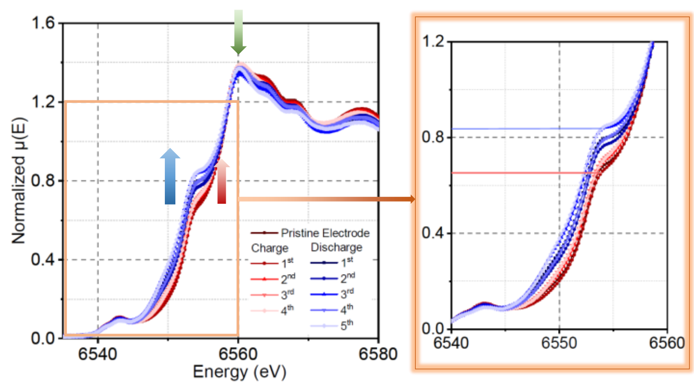
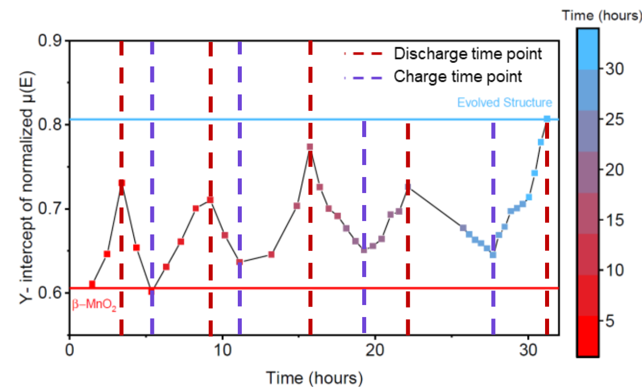
Operando X-ray Absorption Spectroscopy (XAS): Gradual conversion of β-MnO_2 structure

m2m#s molecular to mesoscale



- *Operando* X-ray absorption near edge structure (XANES) vs. the electrochemical potential and reaction time.





- Selected spectra points taken at the end of discharge and charge profiles: the variation in the pre-edge feature
- The Y-intercept of normalized XAS spectra near the pre-edge feature indicating the evolution of structure

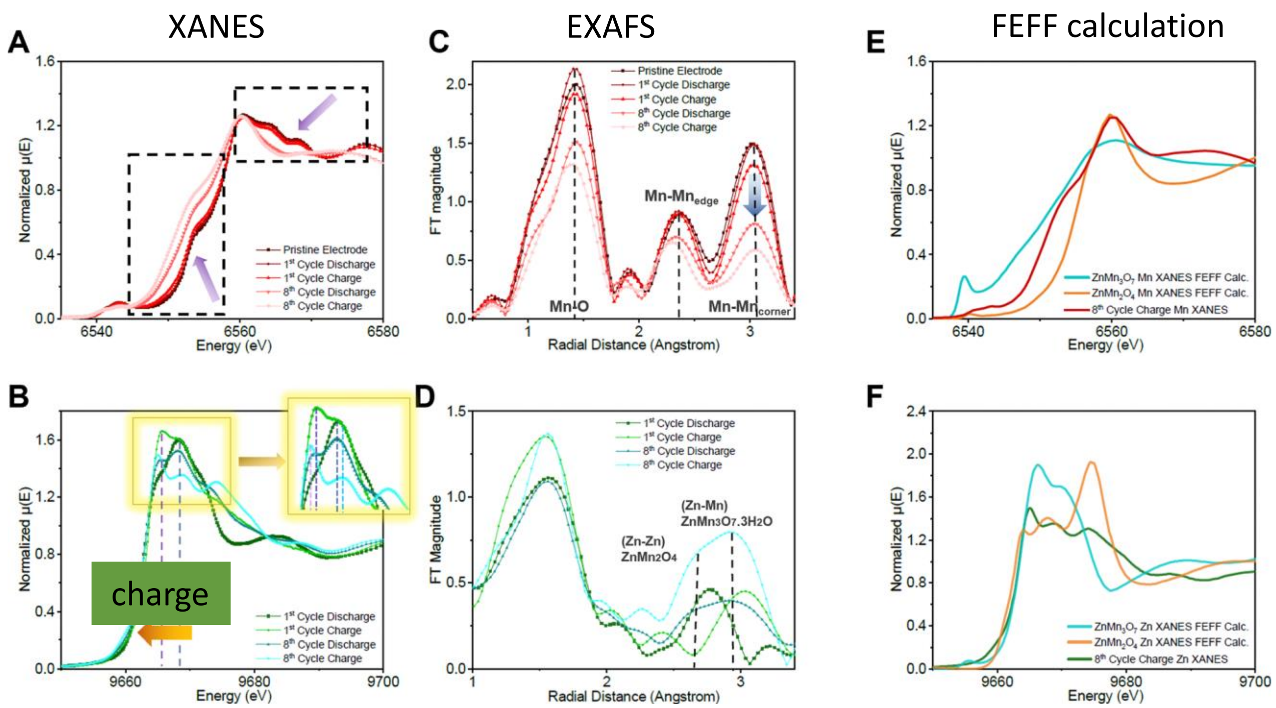
- *Varun R. Kankanallu, Xiaoyin Zheng, Denis Leschev, Nicole Zmich, Charles Clark, Cheng-Hung Lin, Hui Zhong, Sanjit Ghose, Andrew M. Kiss, Dmytro Nykypanchuk, Eli Stavitski, Esther S. Takeuchi, Amy C. Marschilok, Kenneth J. Takeuchi, Jianming Bai, Mingyuan Ge* and Yu-chen Karen Chen-Wiegart, Energy & Environmental Science (2023), DOI: 10.1039/D2EE03731A*

Ex situ XAS of first and eight cycle: discharge and charge

XANES & Extended X-ray Absorption Fine Structure (EXAFS)

Mn K-edge

Zn K-edge



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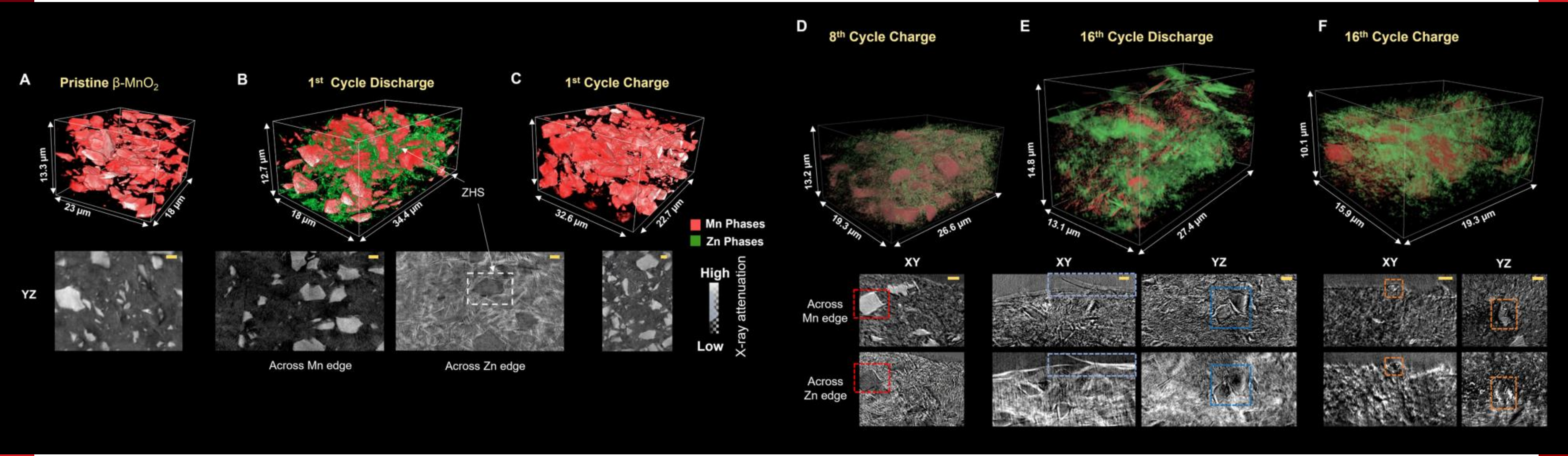
Key morphological features of β-MnO2 electrodes

- **1st cycle discharge:** A dense growth of ZHS precipitate → **reversible upon charge**
- **8th cycle charge:** partial dissolution of β-MnO_2 particles and the Zn–Mn amorphous complex phase
- **16th cycle:** discharge and charge: dissolution of β -MnO_2 and dense growth of Zn phases throughout



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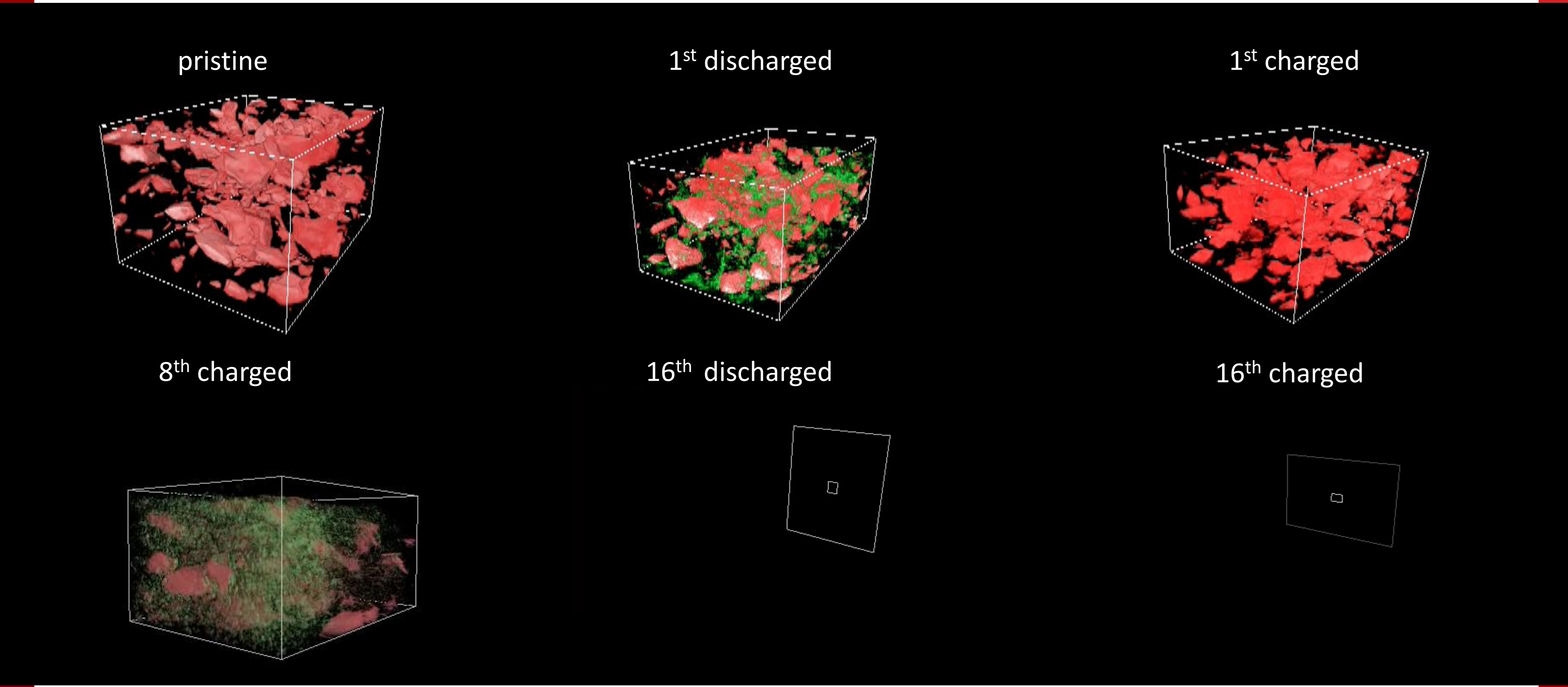
3D morphological and chemical evolution



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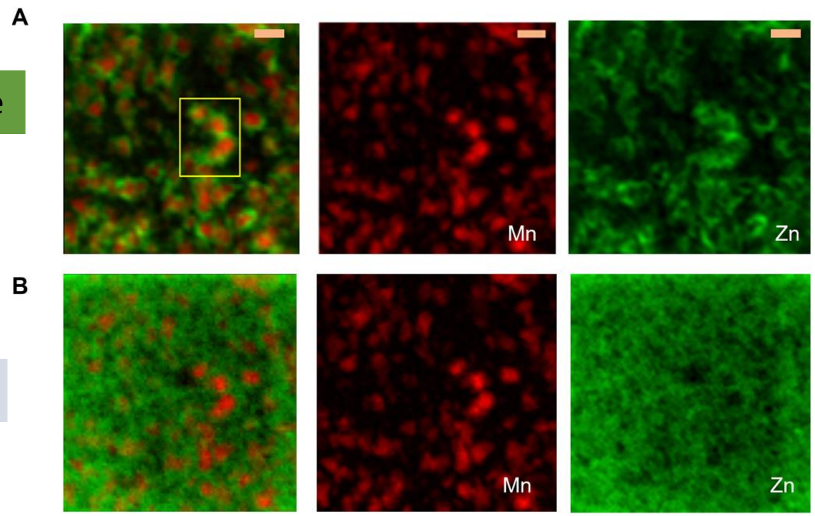
Colocalization of the Zn and Mn phase around the electrode

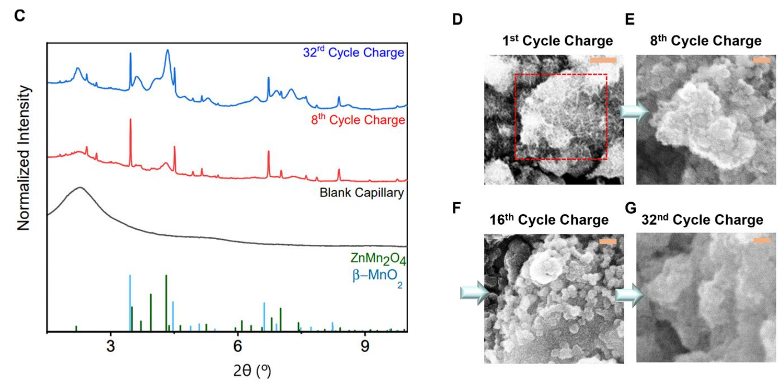
discharge

charge



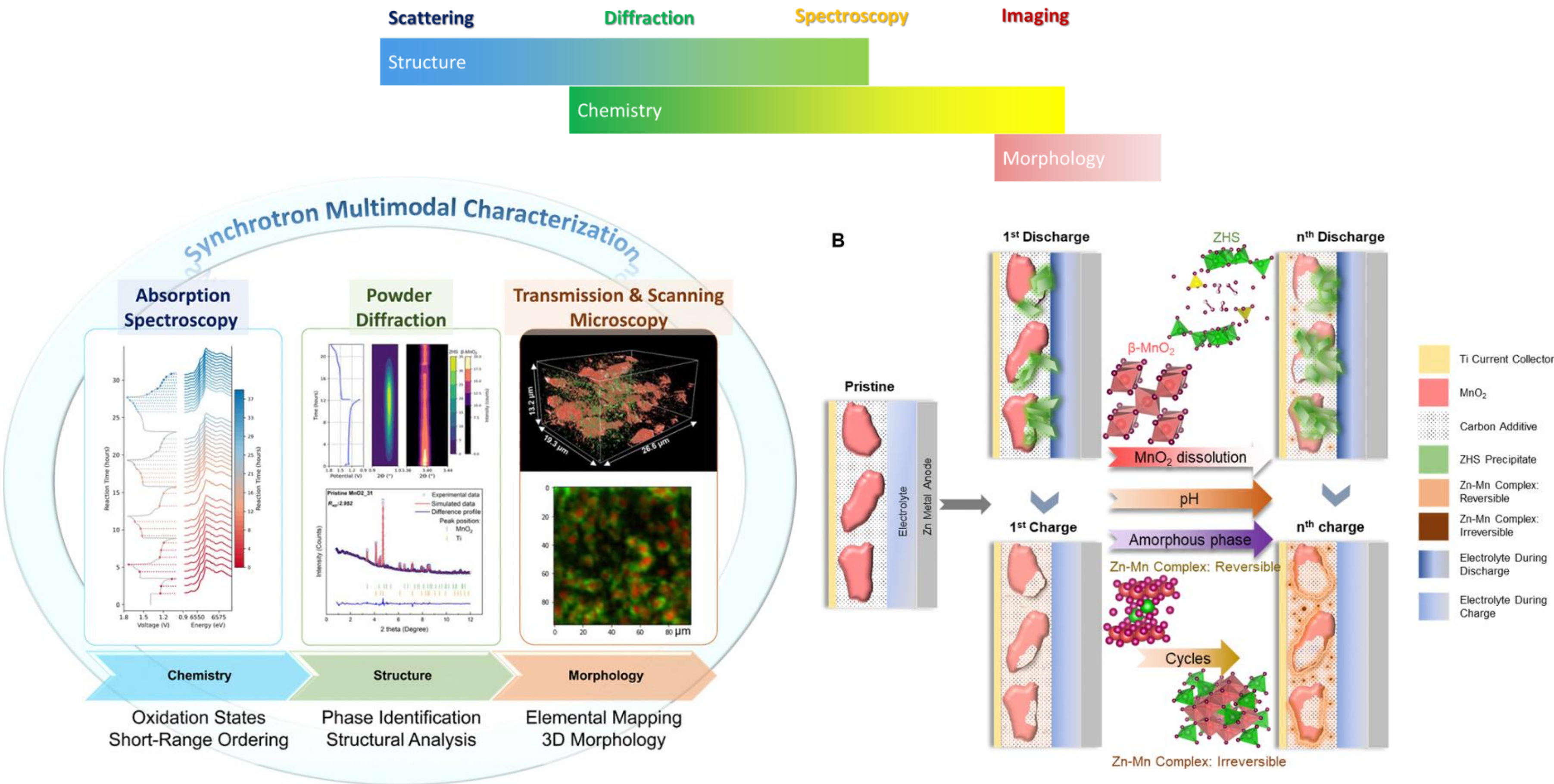
- Colocalization of the Zn phase over the MnO_2 particles (scale bar = 5 micron): ZHS phase formation and reversibility

- Growth of the $ZnMn_2O_4$ phase obtained at the end of 8th and 32nd cycle.
- SEM of 1st cycle at the charged state having a flower like deposition over the MnO_2 particle.
- Growth of spherical round feature, (scale bar = 500 nm, for D = 100 nm)



- *Varun R. Kankanallu, Xiaoyin Zheng, Denis Leschev, Nicole Zmich, Charles Clark, Cheng-Hung Lin, Hui Zhong, Sanjit Ghose, Andrew M. Kiss, Dmytro Nykypanchuk, Eli Stavitski, Esther S. Takeuchi, Amy C. Marschilok, Kenneth J. Takeuchi, Jianming Bai, Mingyuan Ge* and Yu-chen Karen Chen-Wiegart, Energy & Environmental Science (2023), DOI: 10.1039/D2EE03731A*

Proposed reaction mechanism



- *Varun R. Kankanallu, Xiaoyin Zheng, Denis Leschev, Nicole Zmich, Charles Clark, Cheng-Hung Lin, Hui Zhong, Sanjit Ghose, Andrew M. Kiss, Dmytro Nykypanchuk, Eli Stavitski, Esther S. Takeuchi, Amy C. Marschilok, Kenneth J. Takeuchi, Jianming Bai, Mingyuan Ge* and Yu-chen Karen Chen-Wiegart, Energy & Environmental Science (2023), DOI: 10.1039/D2EE03731A*

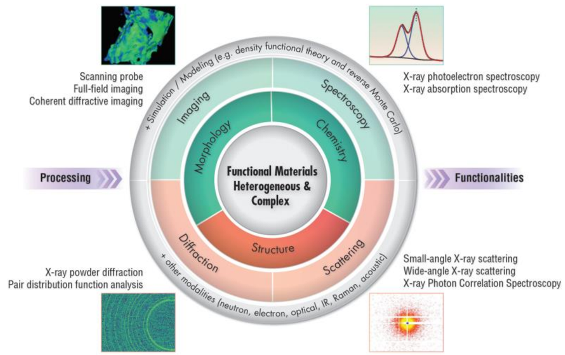
2-Min You Talk!

Talk to your neighbor(s):

1) What is your res … tch")
2) What are the ma … you use to characterize them? (Name at … echnique, if possible!)
3) Why are you usi …

   What informatio … the techniques?

   Are they complementary to each other?

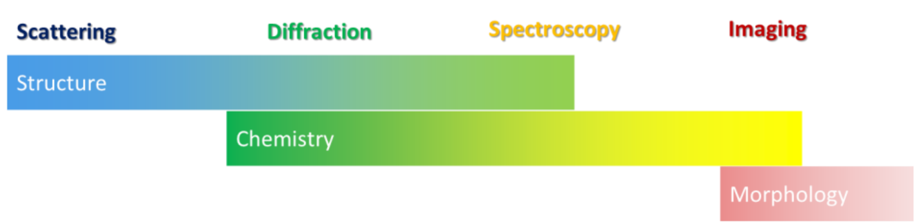


4) **Try to categorize them and see their connections:**

→ Building a mind-map/framework to think/plan your research

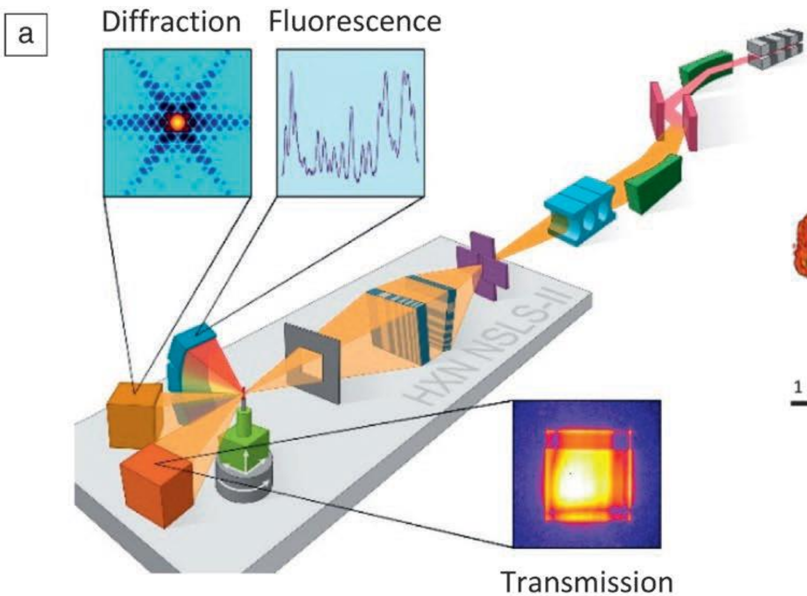
Avoid: I have a hammer, and thus everything looks like a nail!

Ask yourself: why am I using the technique, and what I am trying to get out of it?

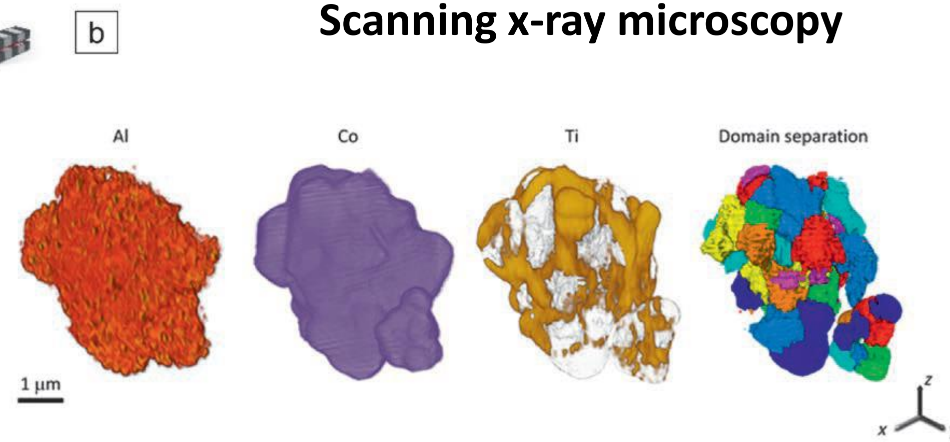


How about for one type of technique?

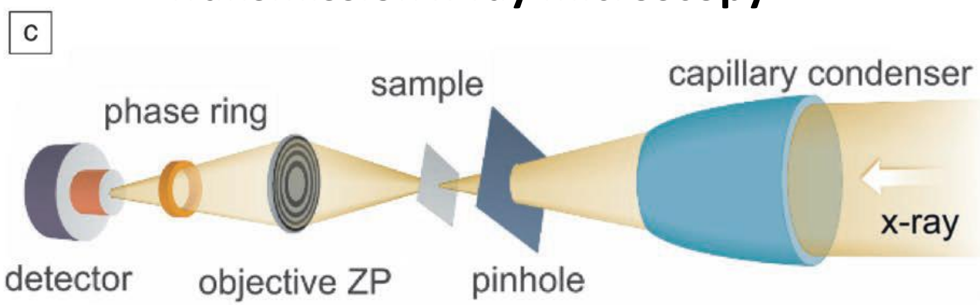
Scanning x-ray microscopy

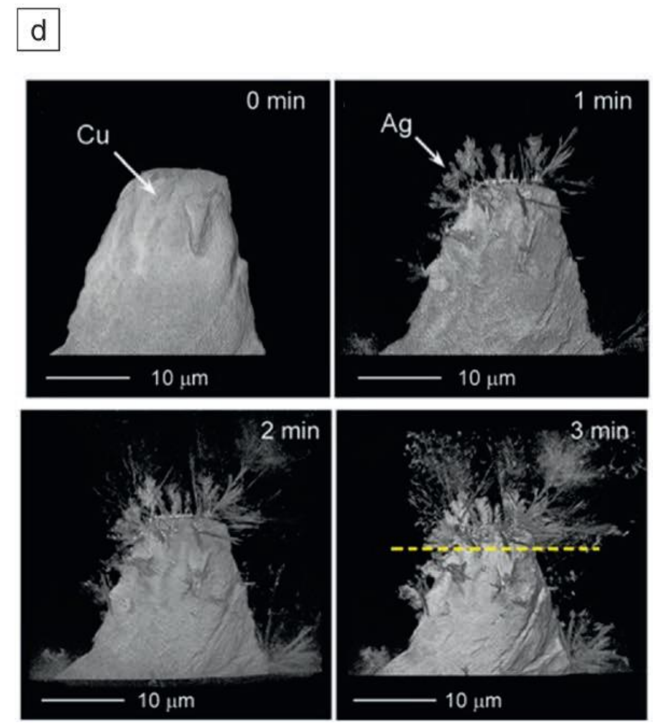


From HXN, 3-ID, NSLS-II



Transmission x-ray microscopy



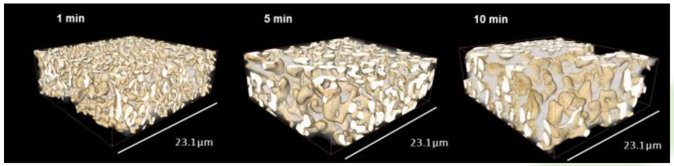


From FXI, 18-ID, NSLS-II

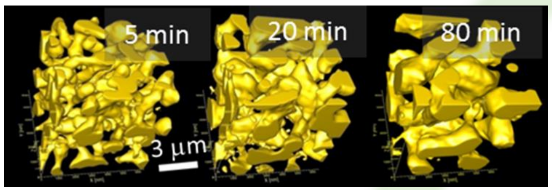
2020 MRS Bulletin, Nanoscale x-ray and electron tomography, Hanfei Yan , Peter W. Voorhees , and Huolin L. Xin , Guest Editors

Modern X-ray Imaging: Multi-dimensional & multimodal

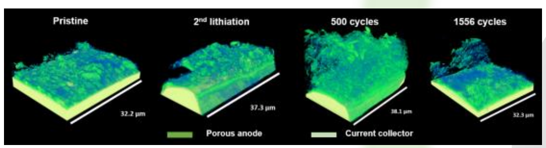
X-ray Imaging & Microscopy



Zhao et al., 2017, ACS App. Mat. & Int.



Chen Wiegart et al., 2012 Acta Mat.



Zhao et al., 2018, Nano Energy

Need 1

3 Dimensional (Spatial) Characterization

Tomography

In situ operando

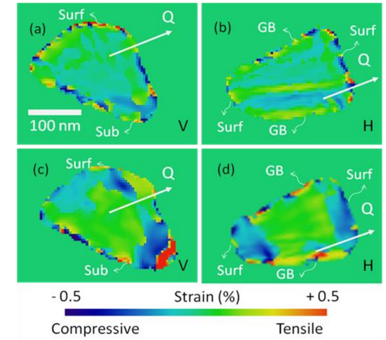
Spectroscopic Imaging

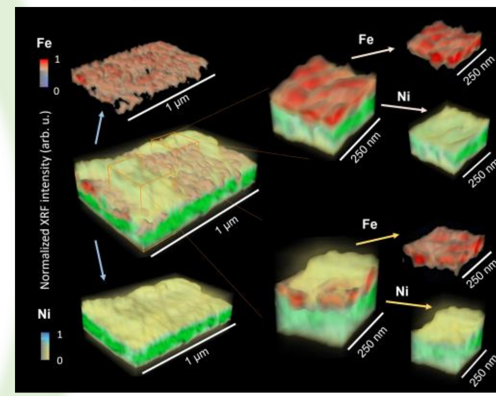
Diffraction Imaging

Need 2

Time-Resolved with Real Environment

Chen Wiegart et al., 2018 Nanoscale





Zhao et al., Materials Horizons, 2019

Need 3

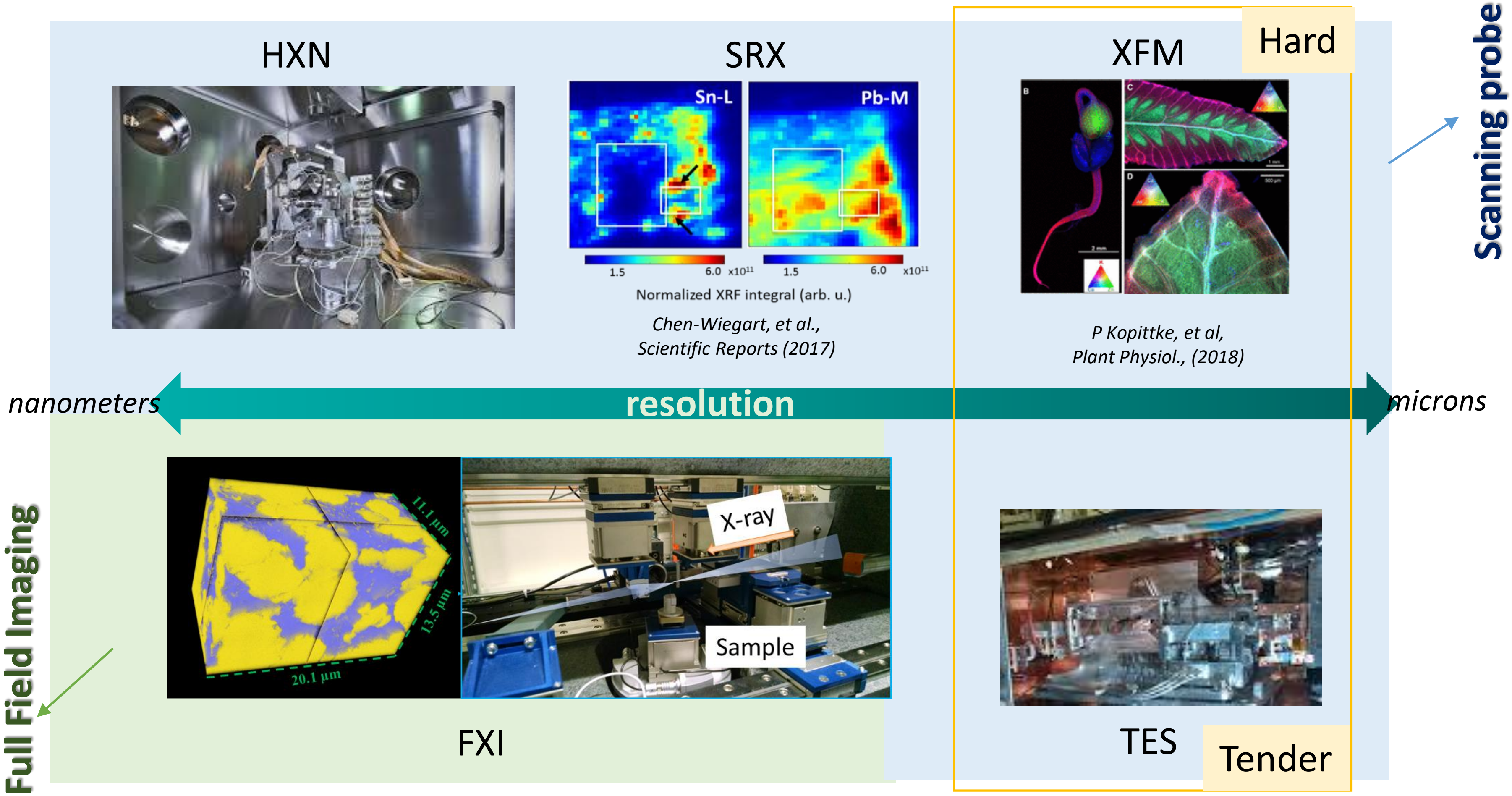
Correlation between Morphology and Other Characteristics: Elemental Distribution, Chemical States, Strain Distribution

Stony Brook University

Karen Chen-Wiegart

Brookhaven National Laboratory

X-ray Microscopy at NSLS-II: A Suite of Tools for Scientific Discovery



- Complementary in resolution, field of view, energy range
- Combination w/ spectroscopy and diffraction analysis

2-Min You Talk!

Talk to your neighbor(s):

1) What is your research topic? (An "elevator pitch")
2) What are the main techniques (2-5 of them) you use to characterize them? (Name at least one X-ray or neutron technique, if possible!)
3) Why are you using them?

   What information can you get out of each of the techniques?

   Are they complementary to each other?
4) Try to categorize them and see their connections:

→ Building a mind-map/framework to think/plan your research

Avoid: I have a hammer, and thus everything looks like a nail!

Ask yourself: why am I using the technique, and what I am trying to get out of it?

5) **Think of other techniques that you may be using in the future that you learned during the X-ray and neutron summer school?**

WIIFM?
What's in it for me?

- What is a multimodal approach?
- Why we care about it?

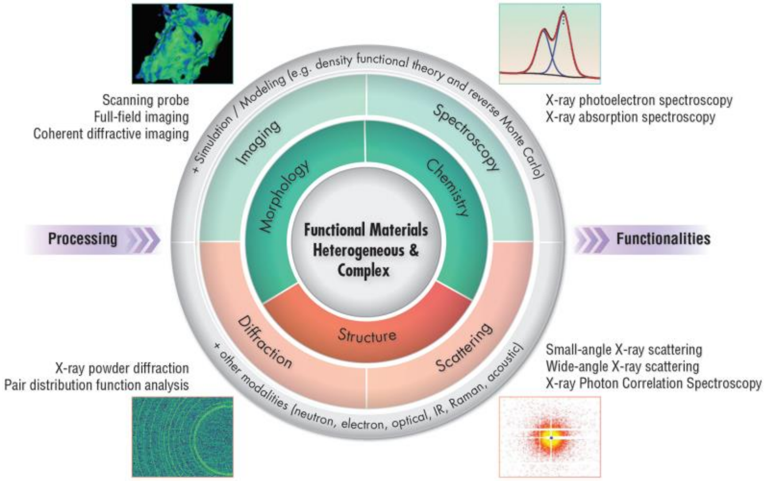
- *Research example: Conversion coating*

- Ways to frame multimodal analysis.

- *Research example: Battery*

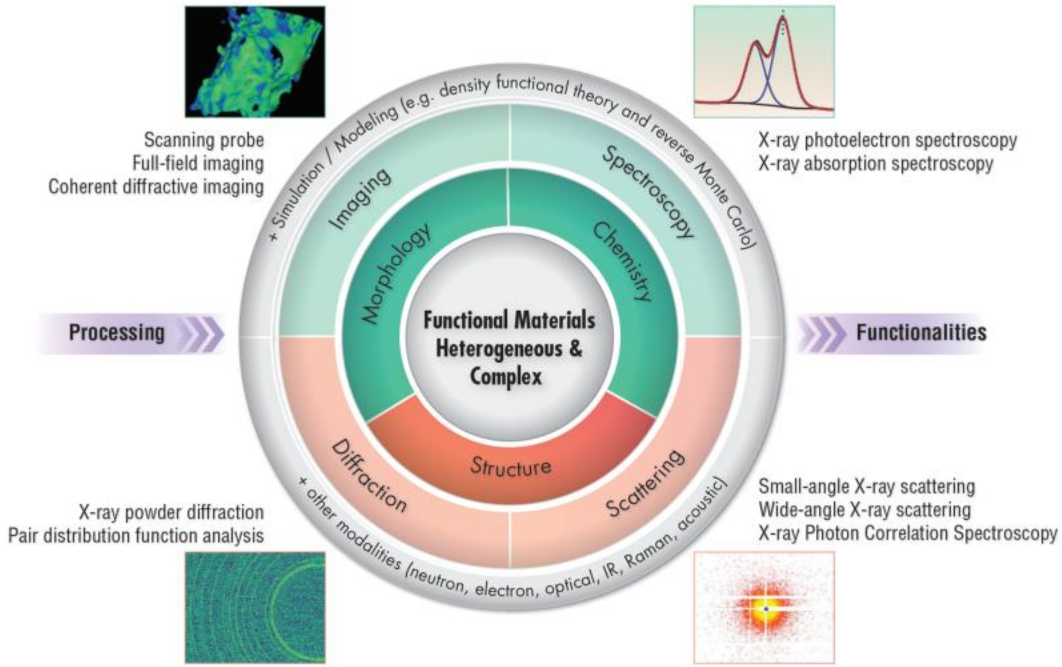
- **Beyond synchrotron**
  - **Other experimental modalities**
  - **Experiment – simulation feedback loop**
  - **Data science opportunities**

- *Research example: Molten Salt and Dealloying*



Beyond Synchrotron

- The synchrotron multimodal approach may be achieved by incorporating ancillary probes into synchrotron beamlines, by exploiting other measurement modalities—such as the electron-based and optical imaging methods—to augment synchrotron datasets, or even by exploiting theory and modeling to complement measurements



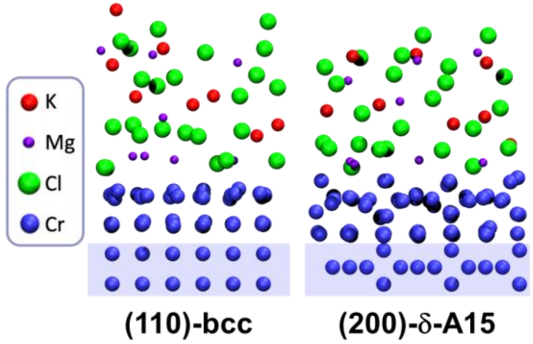
Now broaden it a bit from synchrotron!

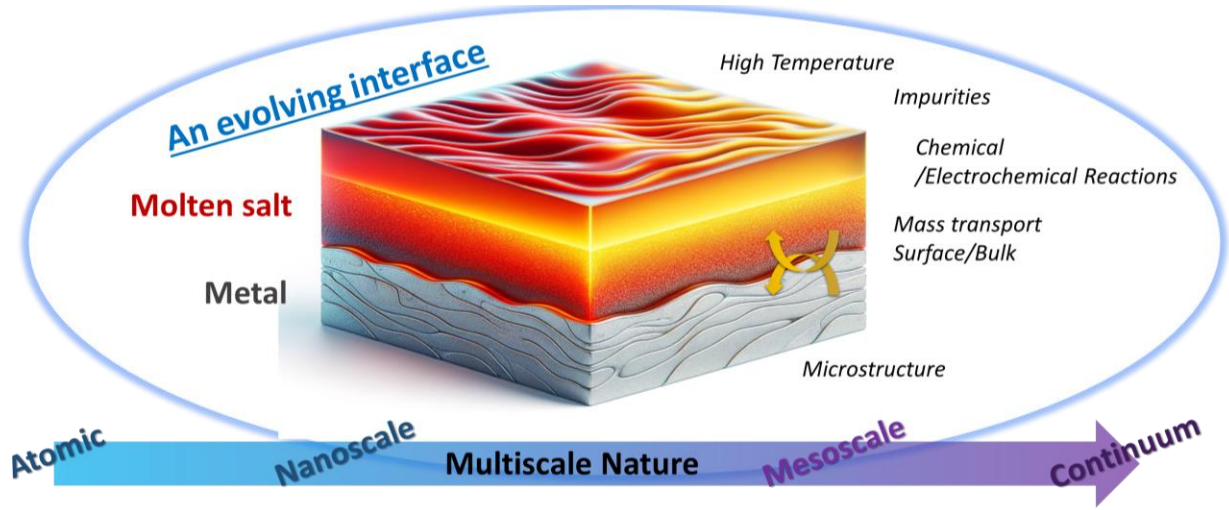
- How do I complement my synchrotron studies?

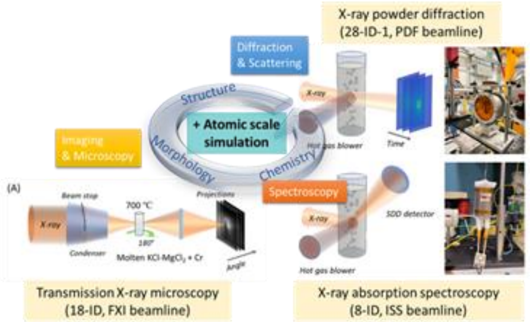
- Lab-based techniques?
  - Pre-characterization?
  - Ex-situ studies to complement the in-situ study?

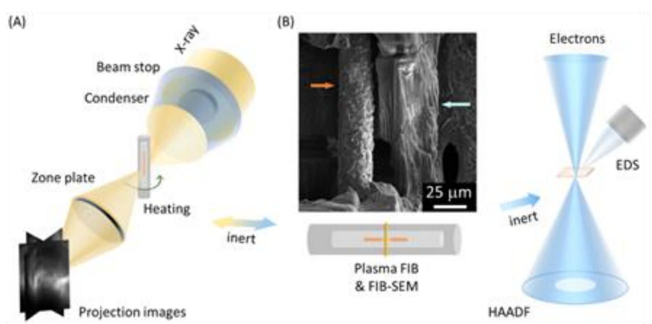
- Other advanced characterizations?
  - E.g. imaging: TEM, Atom-probe, etc.?

- Simulation/modeling/theory?





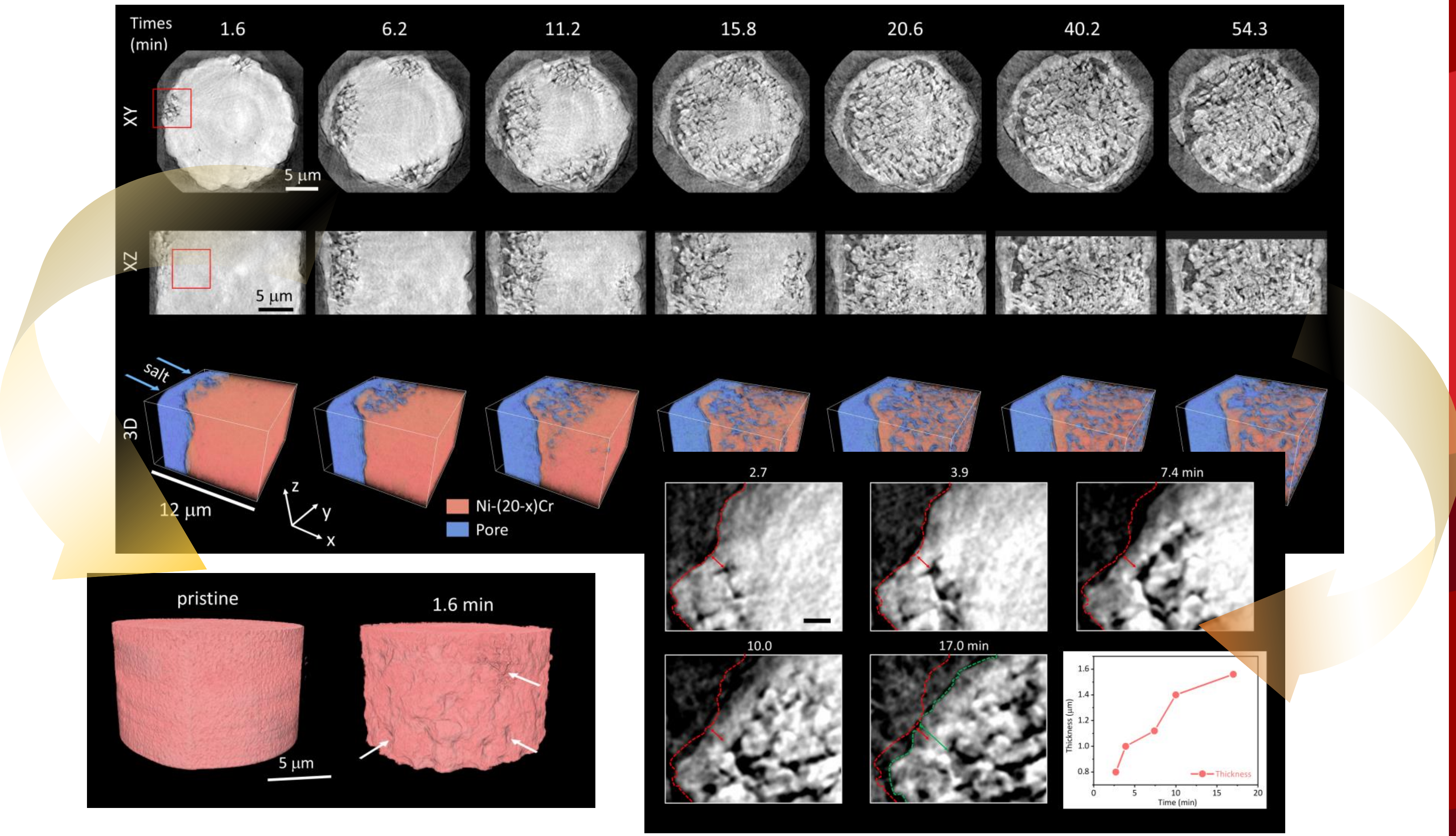




Liu, Chen-Wiegart, et al., ACS Applied Materials & Interfaces (2023)

In situ 3D morphology evolution

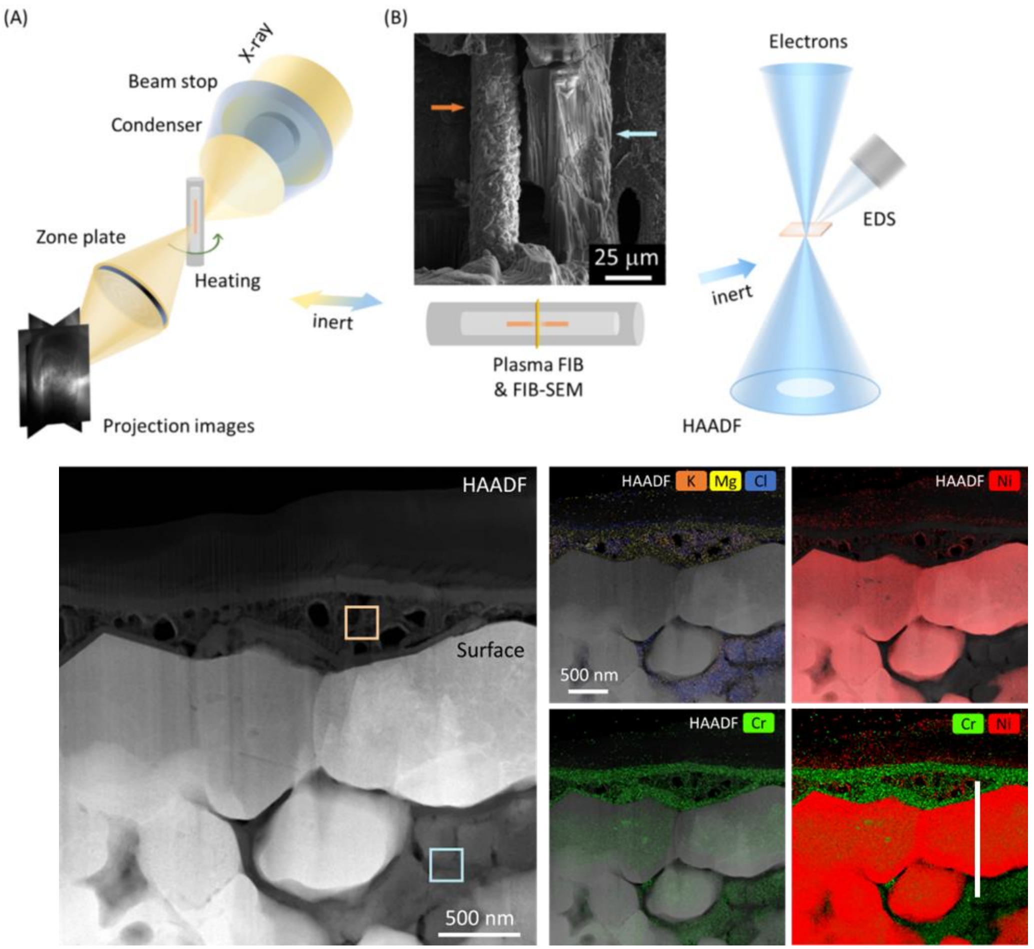
Ni-20Cr reaction in $MgCl_2$-KCl at 600 °C

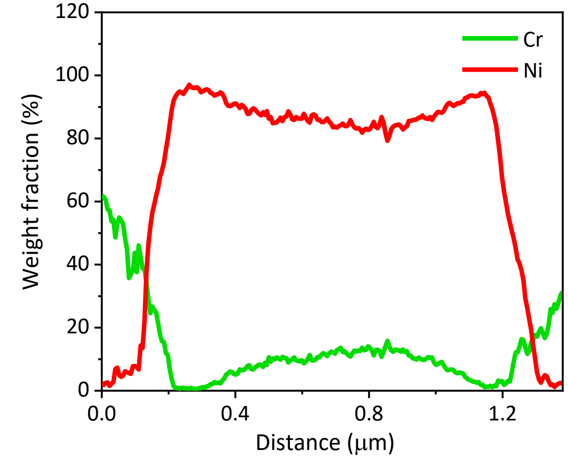


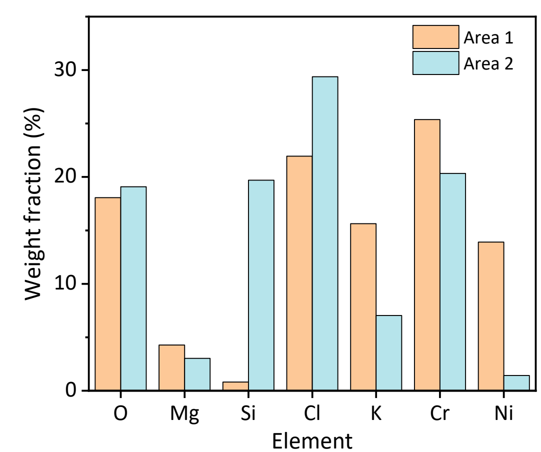
Xiaoyang Liu, Kaustubh Bawane, Karen Chen-Wiegart, *et al., ACS Appl. Mater. Interfaces (2023)*

Elemental Mapping by STEM

Ni-20Cr reaction in $MgCl_2$-KCl at 600 ºC

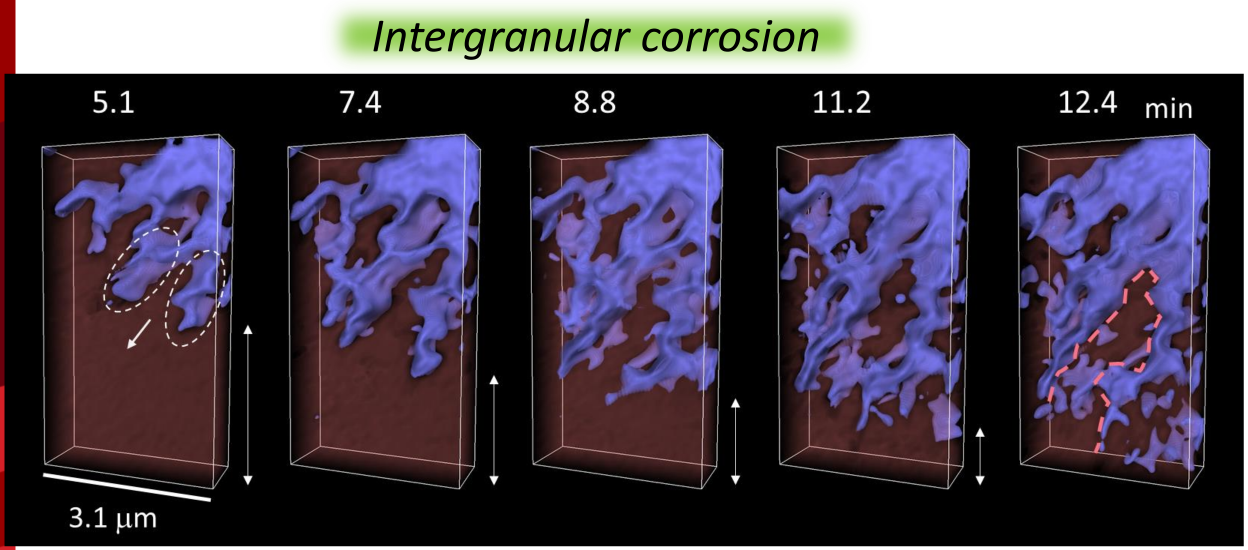


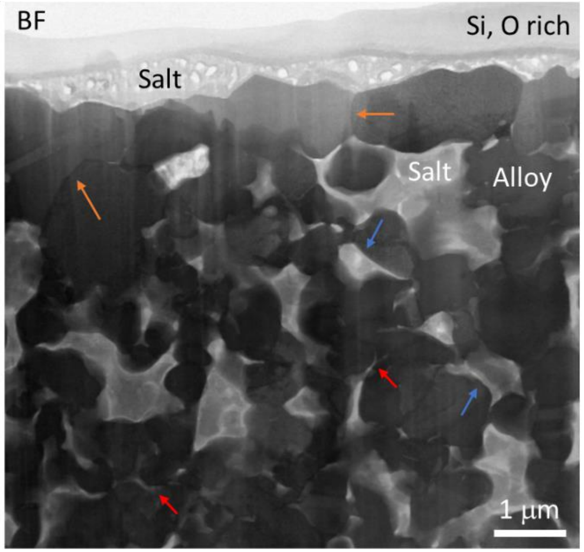


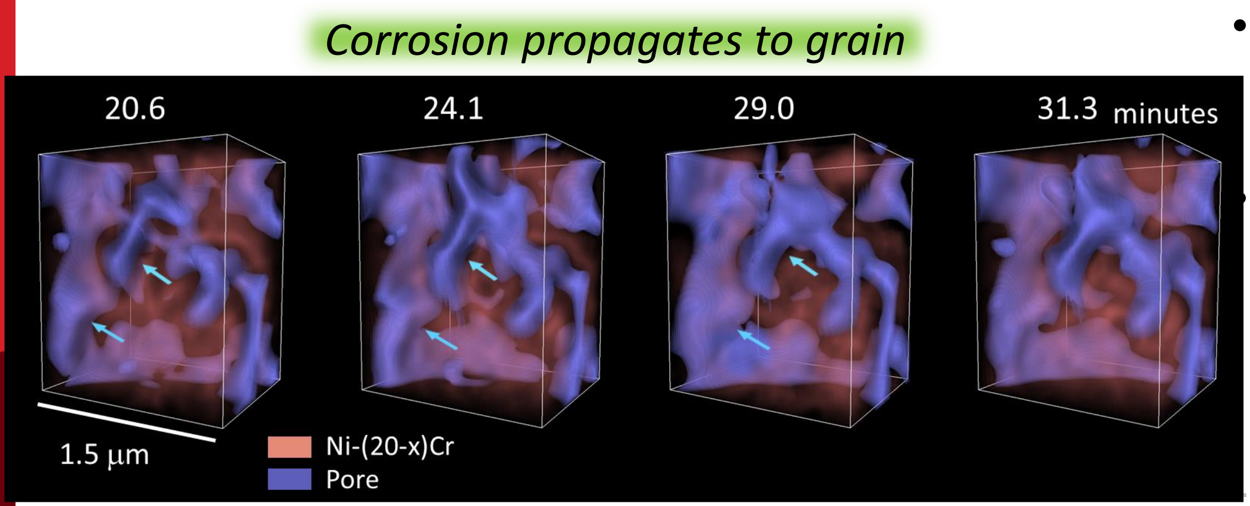


Xiaoyang Liu, Kaustubh Bawane, Karen Chen-Wiegart, *et al., ACS Appl. Mater. Interfaces (2023)*

Multiscale Imaging – X-ray and Electron Microscopy
Ni-20Cr reaction in $MgCl_2$-KCl at 600 °C





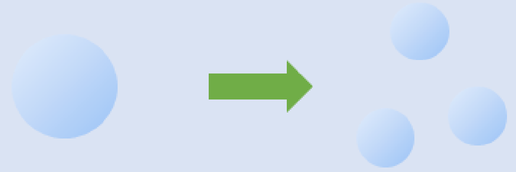


- First corrosion propagates through grain boundary forming cracks
- Corrosion attacks the adjacent grains, enlarging the cracks to large pores

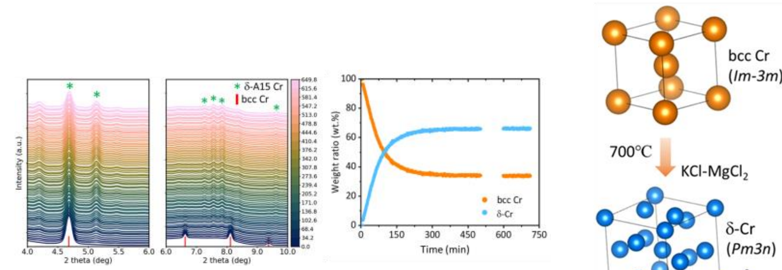
Xiaoyang Liu, Kaustubh Bawane, Karen Chen-Wiegart, *et al., ACS Appl. Mater. Interfaces (2023)*

Probing the Structural and Chemical Evolution of Interfaces in Molten Salt

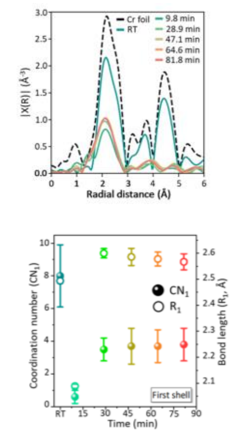
In situ study: Cr microparticles in molten salts



Particle size ↓ Interfacial area ratio ↑

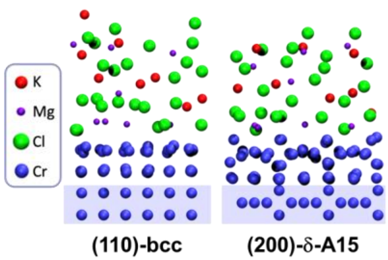


As bcc Cr underwent dissolution, the formation of δ-Cr was observed.

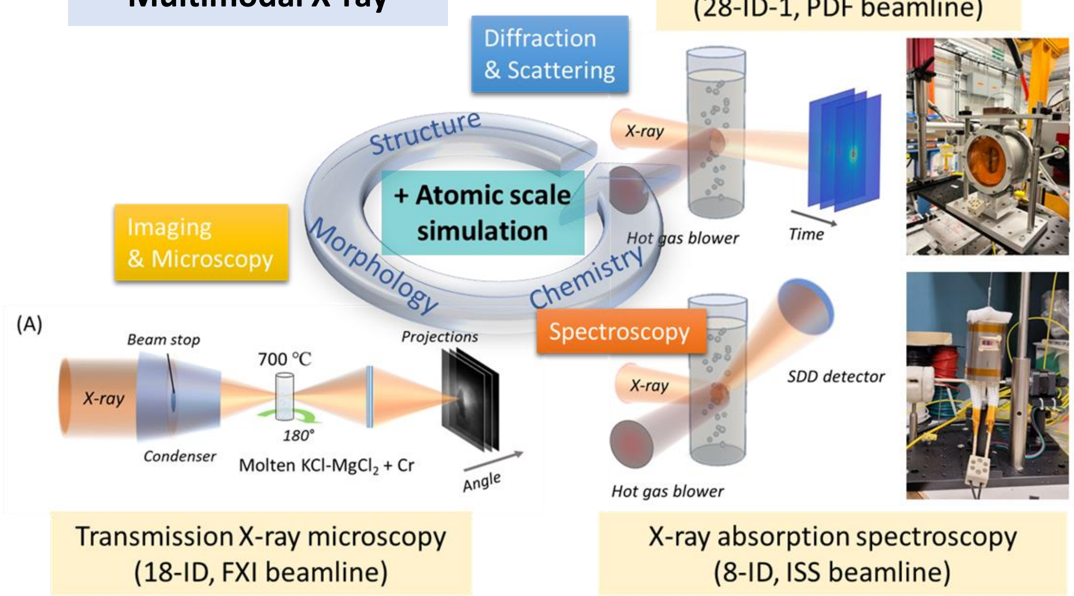


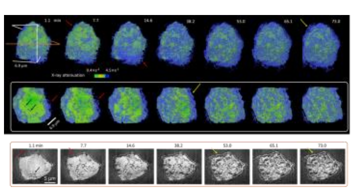
Transformation away from the bcc phase is shown in XAS.

Atomistic Simulation



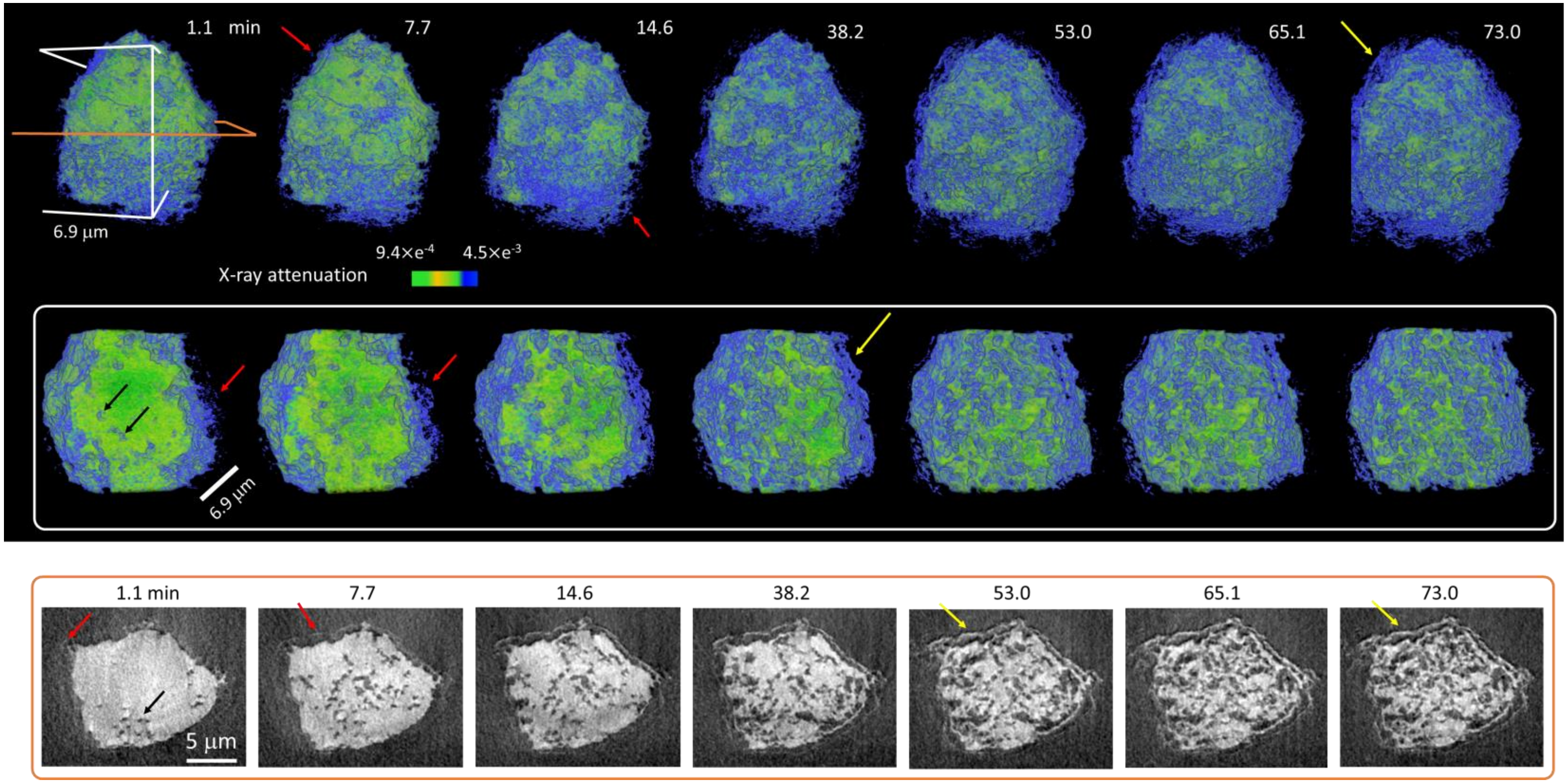
Multimodal X-ray





The dissolution of Cr resulted in the formation of 3D pores

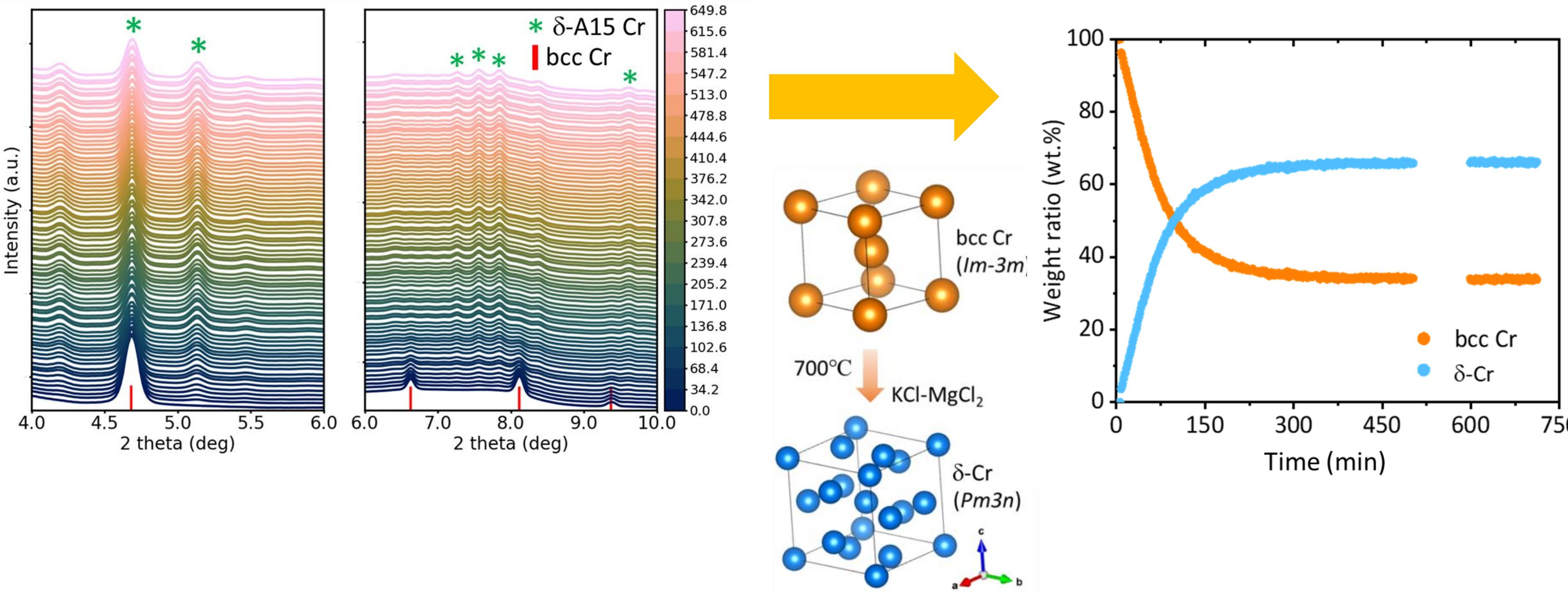
Multimodal Synchrotron Analysis:
In situ X-ray Nano-tomography – 3D Morphological Evolution



- The dissolution of Cr resulted in the formation of 3D pores, leading to a decrease in volume, an increase in surface area, and an elevated surface-to-volume ratio.
- A layer developed on the surface of the Cr particle, characterized by the expansion of the particle's contour during heating.

Liu, Chen-Wiegart, et al., Physical Chemistry Chemical Physics (2024)

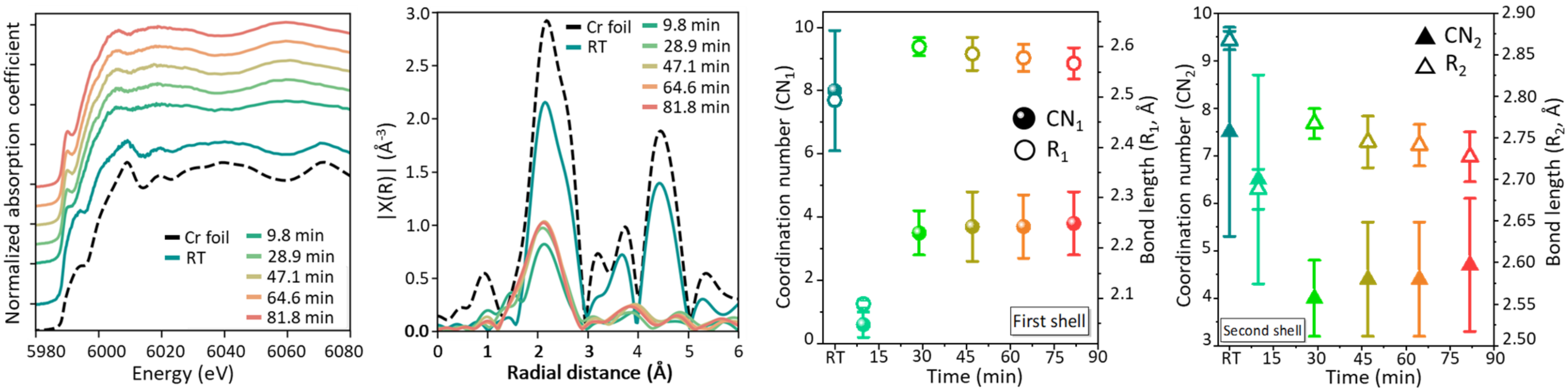
Multimodal Synchrotron Analysis:
In situ X-ray Diffraction – Crystalline Structural Change

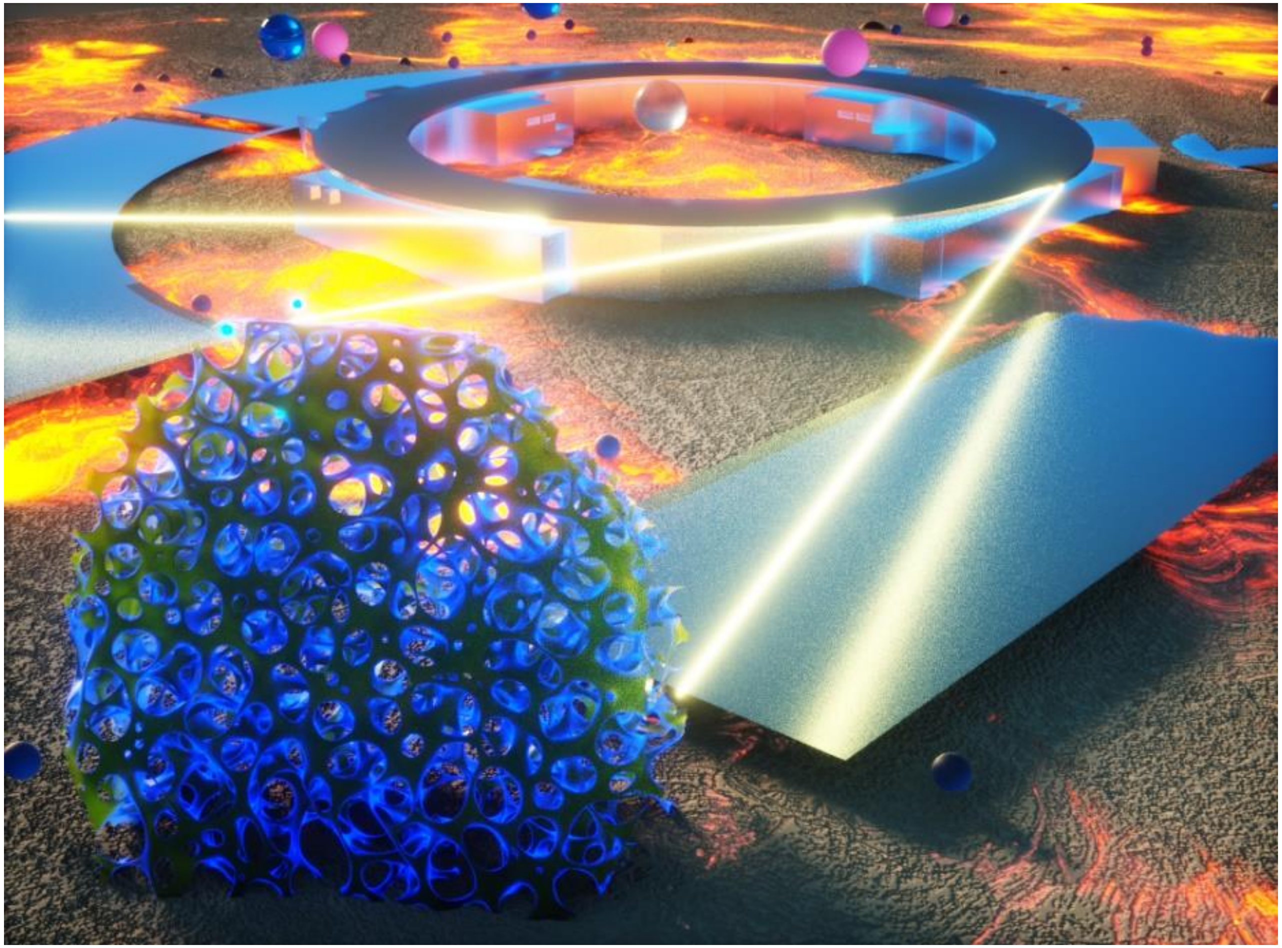


- As bcc Cr underwent dissolution, its peaks disappeared, accompanied by a decrease in the relative weight ratio over time as heating progressed.
- The formation of δ-Cr corresponds to an increase of its characteristic peaks and an increase in the relative weight ratio as a function of time during heating.

Multimodal Synchrotron Analysis:
In situ X-ray Absorption Spectroscopy –
Short-Range Ordering and Chemical Environment Changes

- The evolving XANES features, coordination numbers (CN) and bond lengths (R1, R2) indicate a transformation away from the bcc phase, and a formation of a nanoscale, δ-Cr structure.

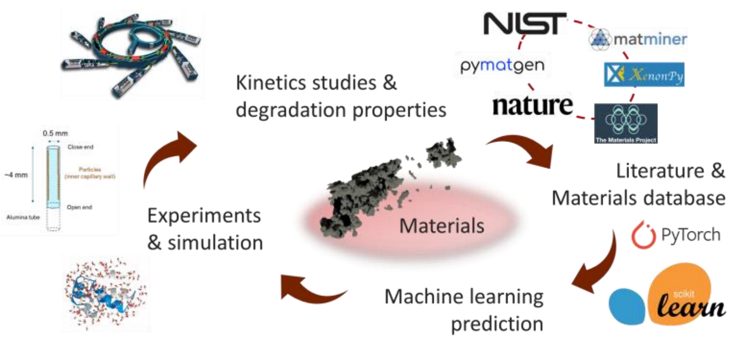




Artwork illustrating the concept of probing the interfaces between molten salts and materials using multimodal synchrotron X-ray techniques and atomistic simulations. ***Selected as a front cover in PCCP.***

Multimodal synchrotron experiments and involving AI-agent in synchrotron experiments

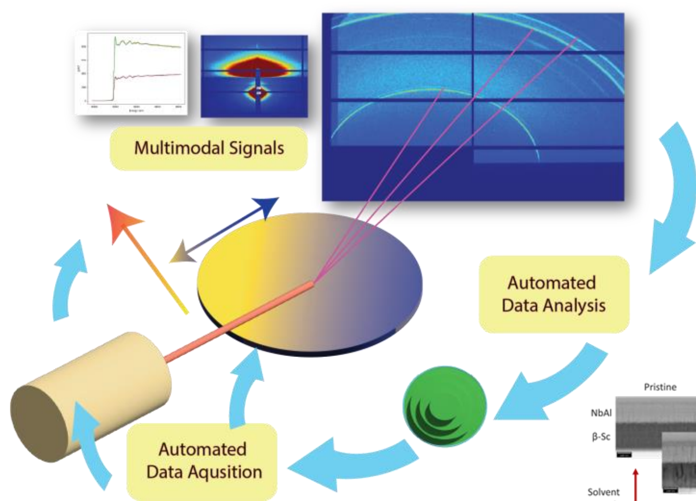
Closed-loop Materials Design

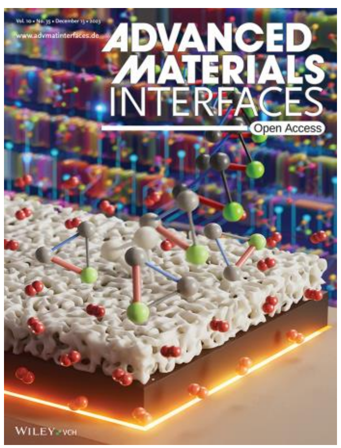


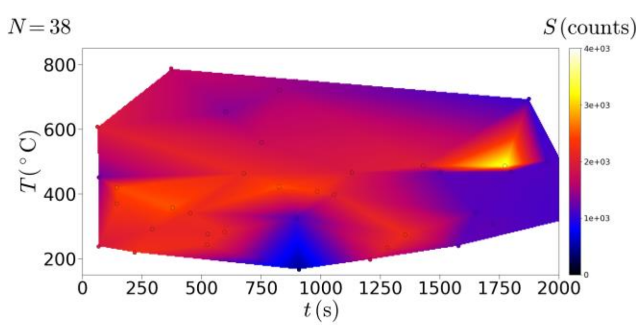
Revised Concept Figure by Cheng-Chu Chung

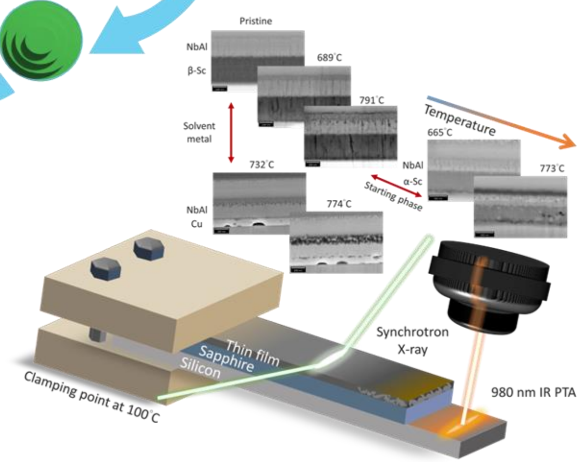
Zhao, C. Chen-Wiegart, K. et al. Commun Mater (2022).

Synchrotron Autonomous Experiment







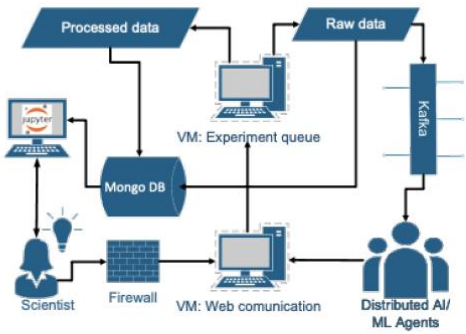


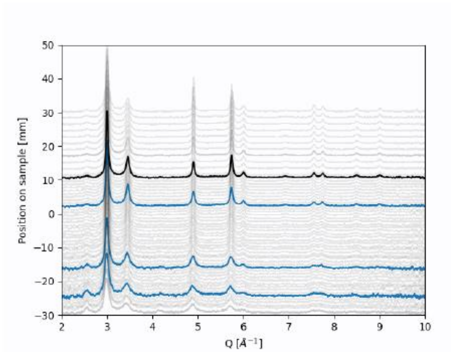
Chung, Chen-Wiegart, et al., Advanced Materials Interfaces (2023)

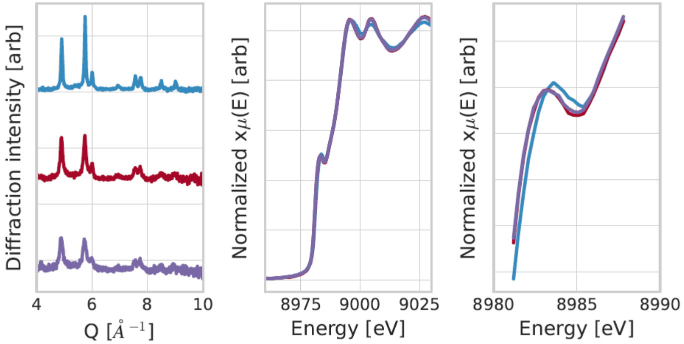
Image Credit: Cheng-Chu Chung

- Real-time analysis and control of multiple beamlines simultaneously
    - Identical sample wafers loaded at BMM and PDF beamlines

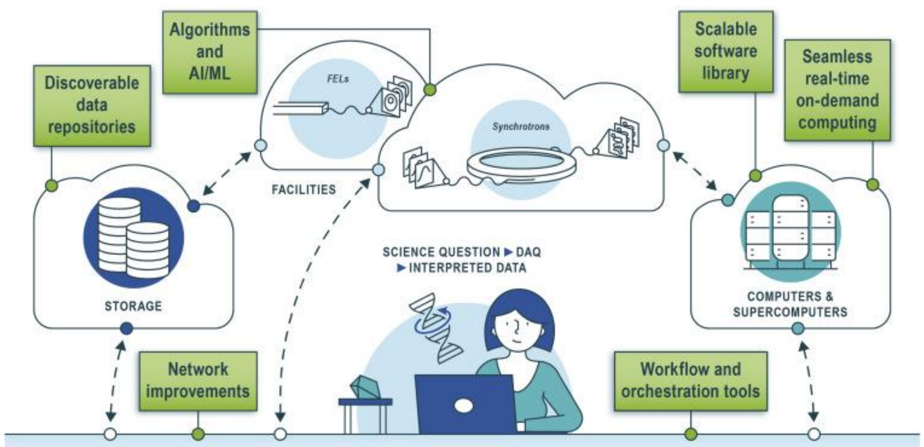
Measuring diffraction (fast) >> apply ML analysis >> select points for measuring spectroscopy (slow)

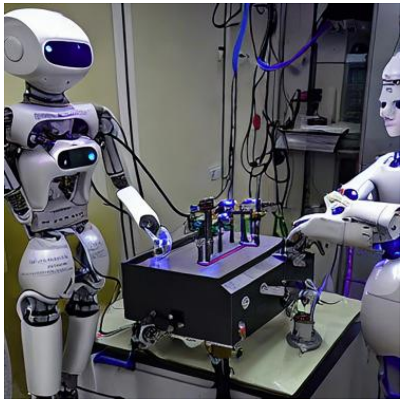


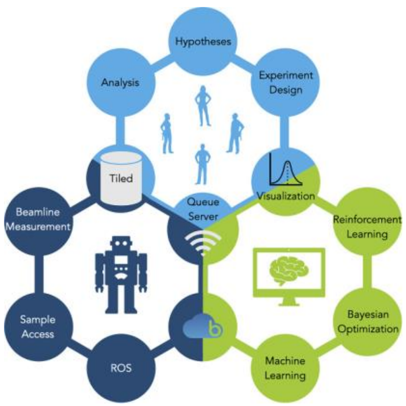




Maffettone, Ravel, Olds, et al., 36th Conference on Neural Information Processing Systems (NeurIPS 2022).

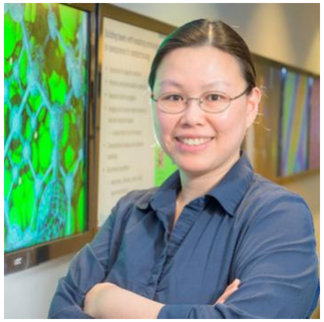






Maffettone, et al., Cell Reports Physical Science, 2022

More references



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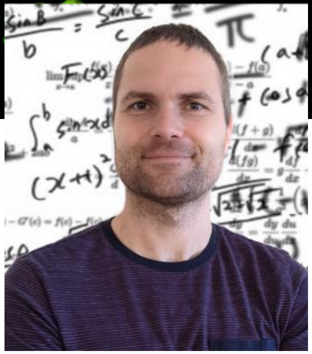

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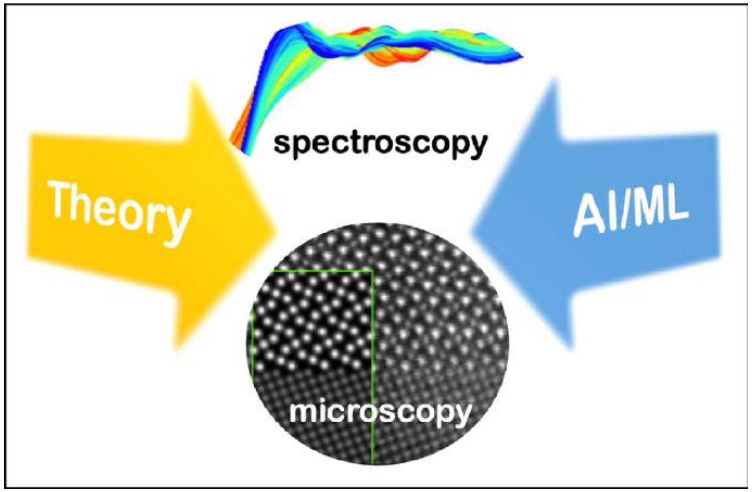
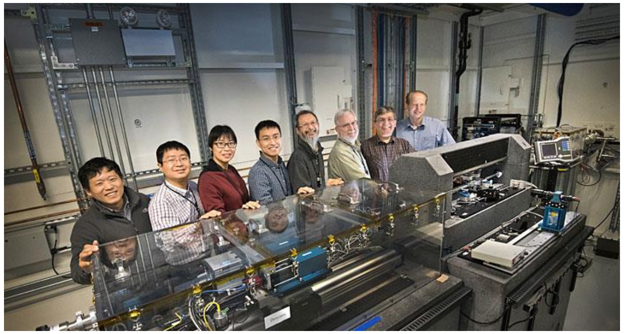
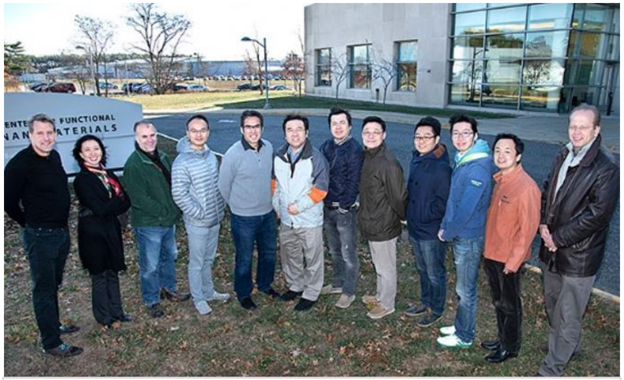
https://autonomous-discovery.lbl.gov/



Theory+AI/ML for microscopy and spectroscopy: Challenges and opportunities Davis Unruh, Venkata Surya Chaitanya Kolluru, Arun Baskaran, Yiming Chen & Maria K. Y. Chan MRS Bulletin (2022) https://doi.org/10.1557/s43577-022-00446-8

Acknowledgements





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PDF: Daniel Olds
XPD: Jianming Bai, Sanjit K. Ghose, Hui Zhang
ISS: Eli Eli Stavitski, Denis Leshchev
BMM: Bruce Ravel
CHX: Lutz Wiegart

CFN, BNL

Kim Kisslinger, Ming Lu, Fernando Camino,Mingzhao Liu, Gwen Wright

SBU

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Thank YOU!!

Chen-Wiegart Group at Stony Brook University

NXS Lecture - Yu-Chen Karen Chen-Wiegart: Multi-modal experiments

Feedback? ☺