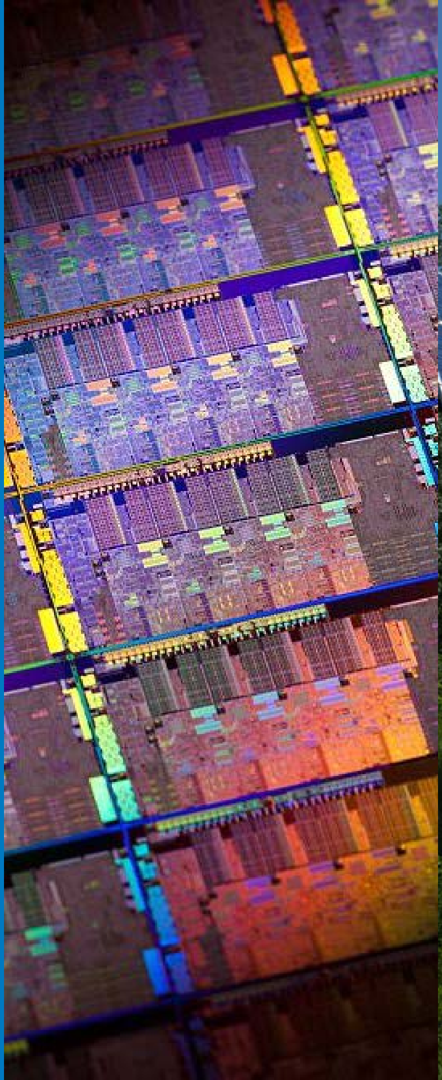
NREL
Transforming ENERGY

University of Colorado Boulder

Beyond Human Vision
Exploring Materials with Machine Intelligence

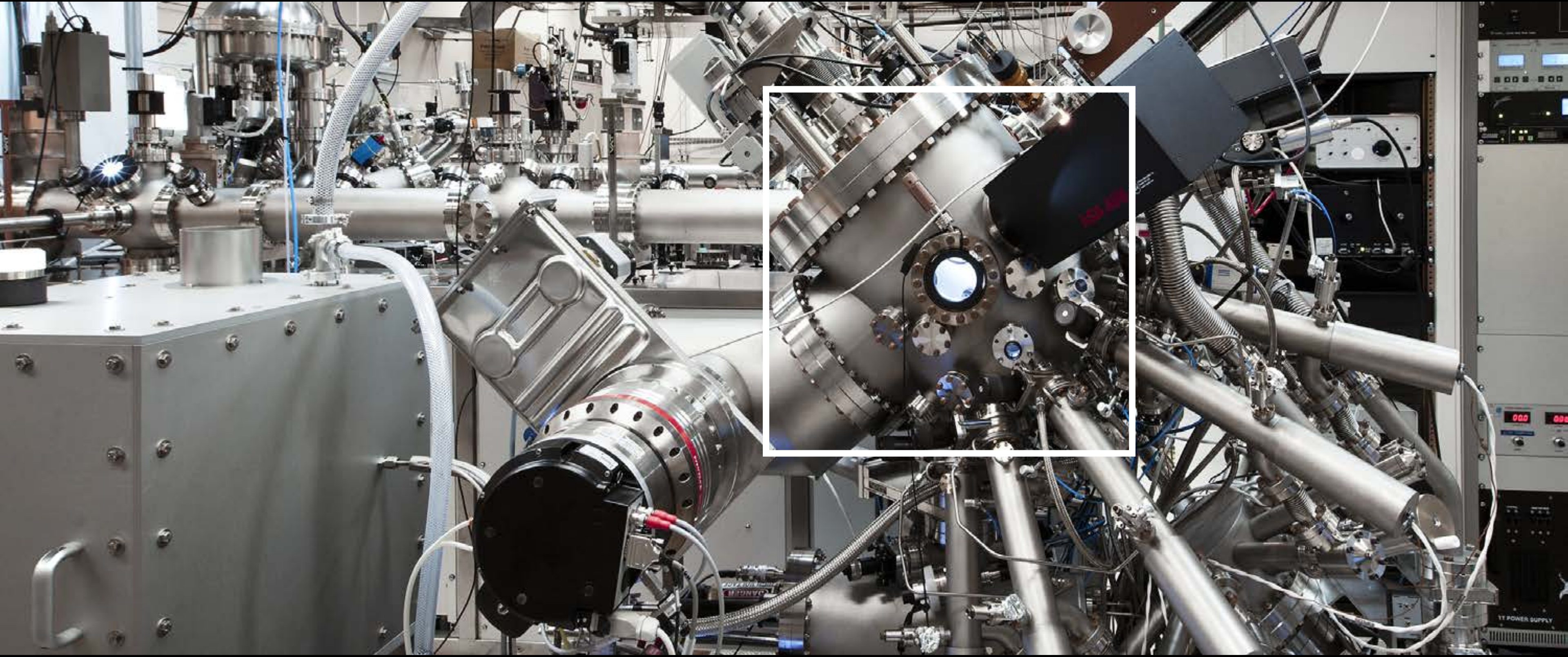
Steven R. Spurgeon
MSSEM Fall Meeting 2024
November 6, 2024

Everyday technologies are critically reliant on mastering materials lifecycles



Wafer: Intel Company
Array / SOFC: NREL

Mastery depends on understanding of complex synthesis pathways…



Oxide Epitaxy Lab @ PNNL

Mastery depends on understanding of complex synthesis pathways…

Kaganer. Paul Drude Institute.

…and degradation behavior in real-world extreme environments.

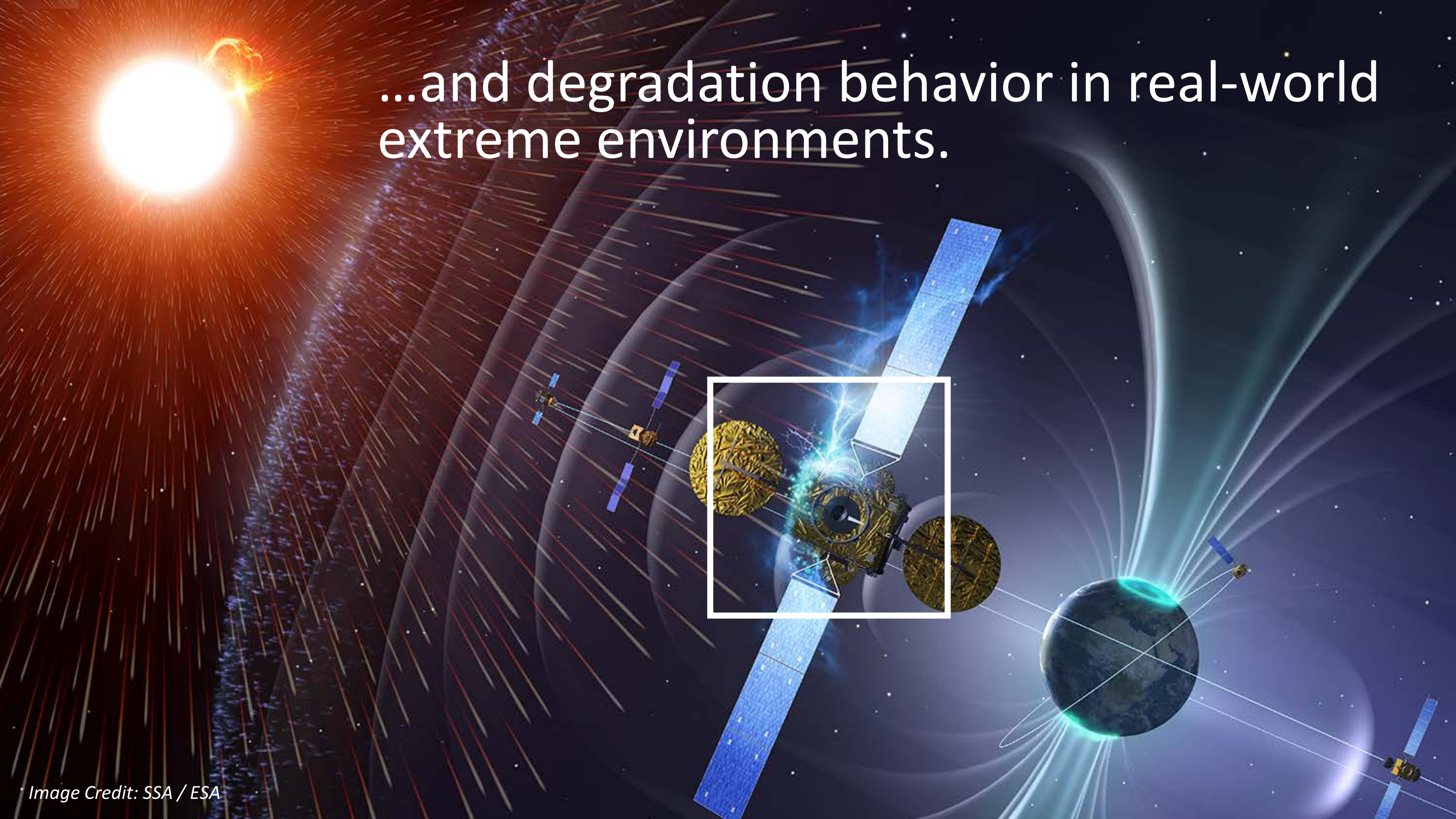
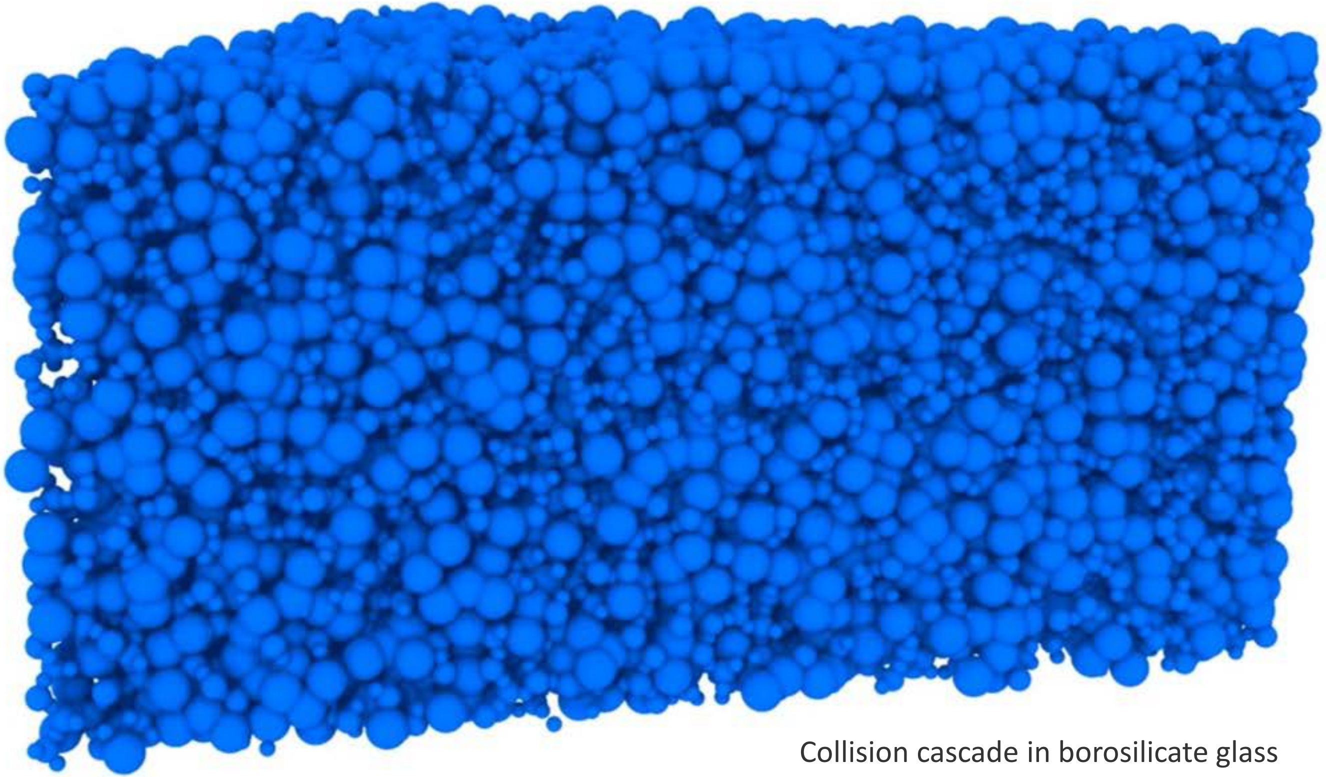


Image Credit: SSA / ESA

…and degradation behavior in real-world extreme environments.

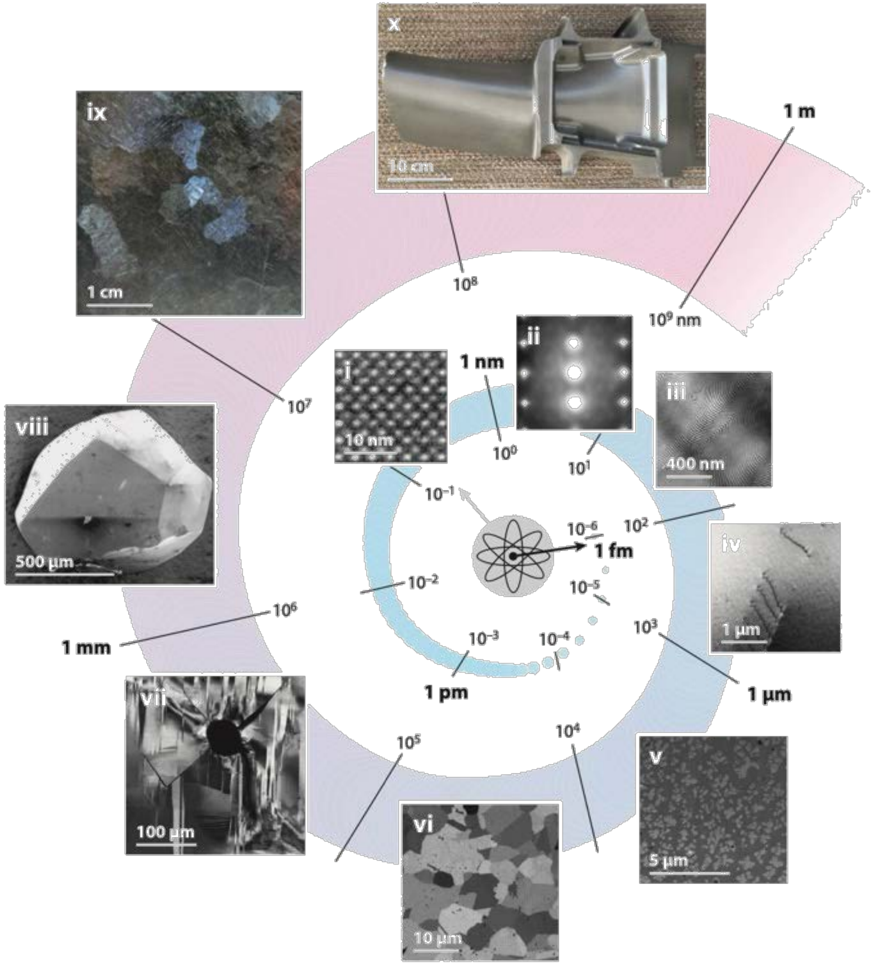


Collision cascade in borosilicate glass

D.A. Kilymis et al. J Non-Cryst Solids. 432, 354-360 (2016).

My research aim is an ontology of the materials lifecycle:

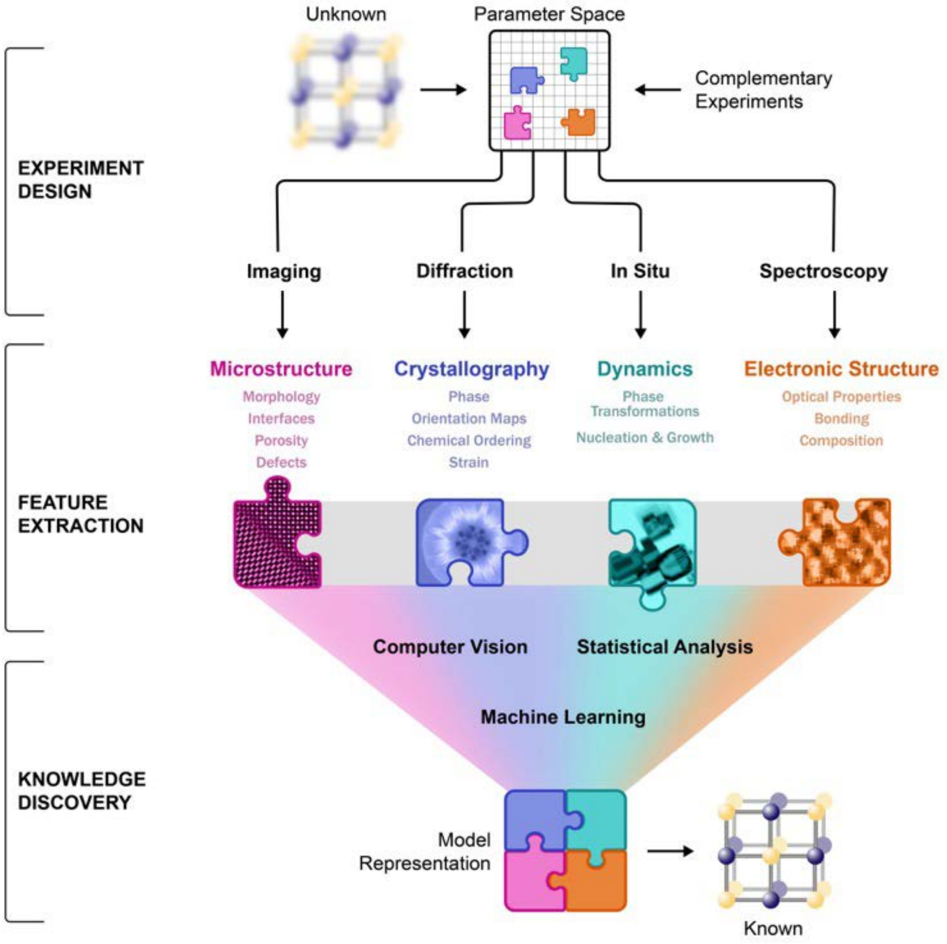
“A systematic mapping of data to meaningful semantic concepts…” ***across spatial and temporal scales***



Kalidindi et al. Ann. Rev. Mater. Res. 45: 171-193. (2015).

Quote adapted from: https://blog.palantir.com/ontology-finding-meaning-in-data-palantir-rfx-blog-series-1-399bd1a5971b

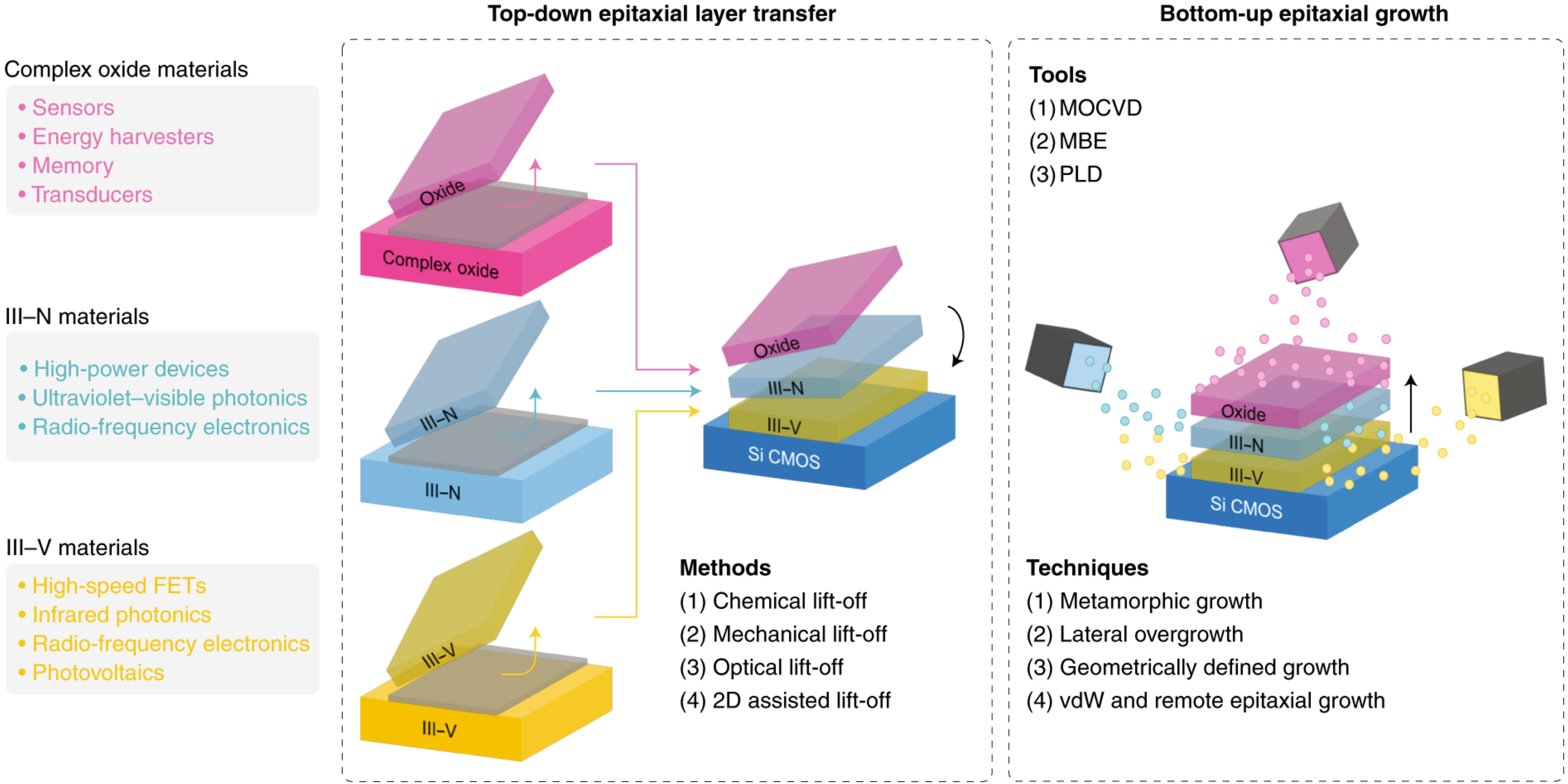
Autonomous science plays an important role in developing and harnessing this ontology



Spurgeon et al. Nature Mater, 20(3), 274–279. (2021).

Understanding Materials Synthesis

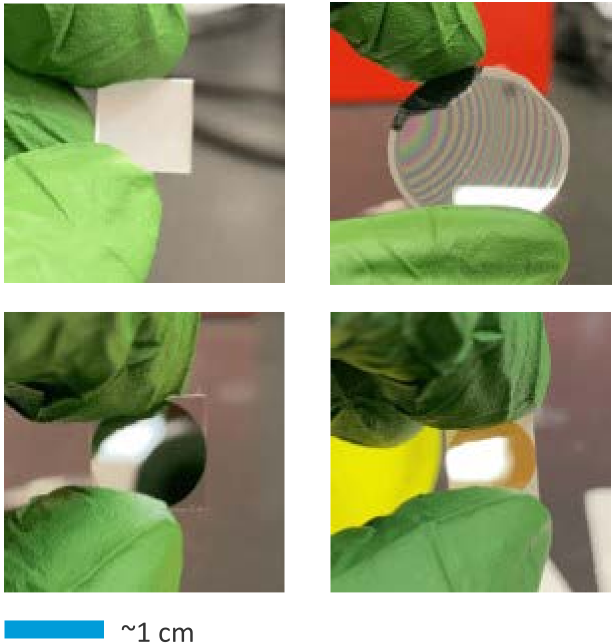
Epitaxial integration of semiconductors and oxides is a challenge for emerging devices



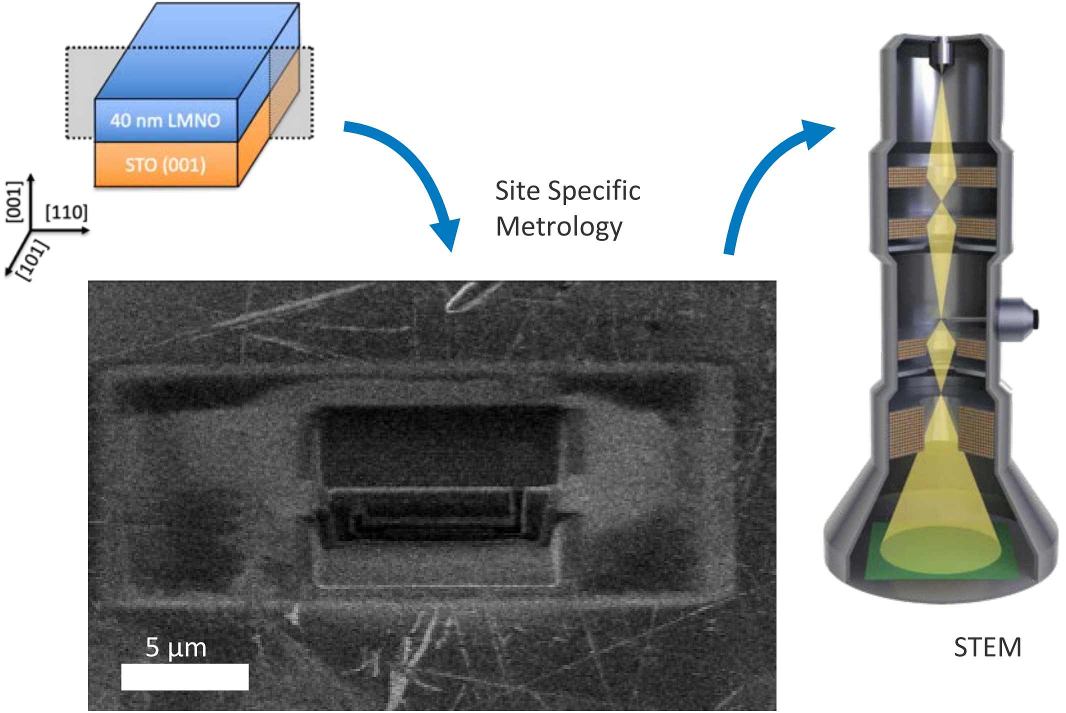
Kum et al. Nature Electron. 2, 439–450 (2019).

Tailored materials design requires direct local probes of structure and chemistry

Functional Thin Films for Energy Applications



~1 cm

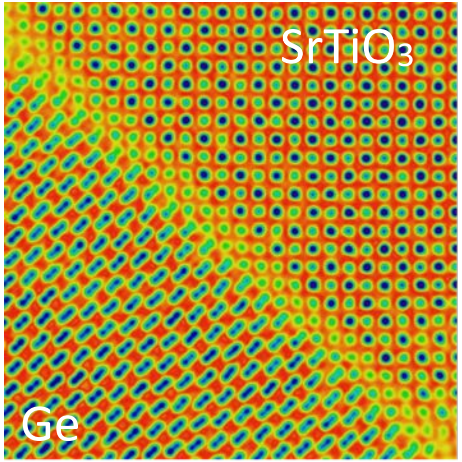


Focused Ion Beam

Spurgeon et al. Chem Mater, 28.11. 3814–3822. (2016).

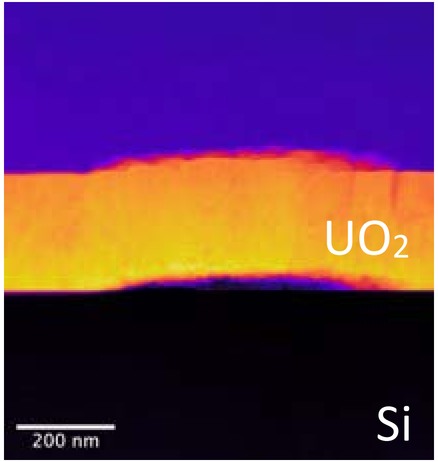
Electron microscopy can richly inform lifecycle models to achieve predictive control

Structure → **Chemistry**



Imaging

Diffraction

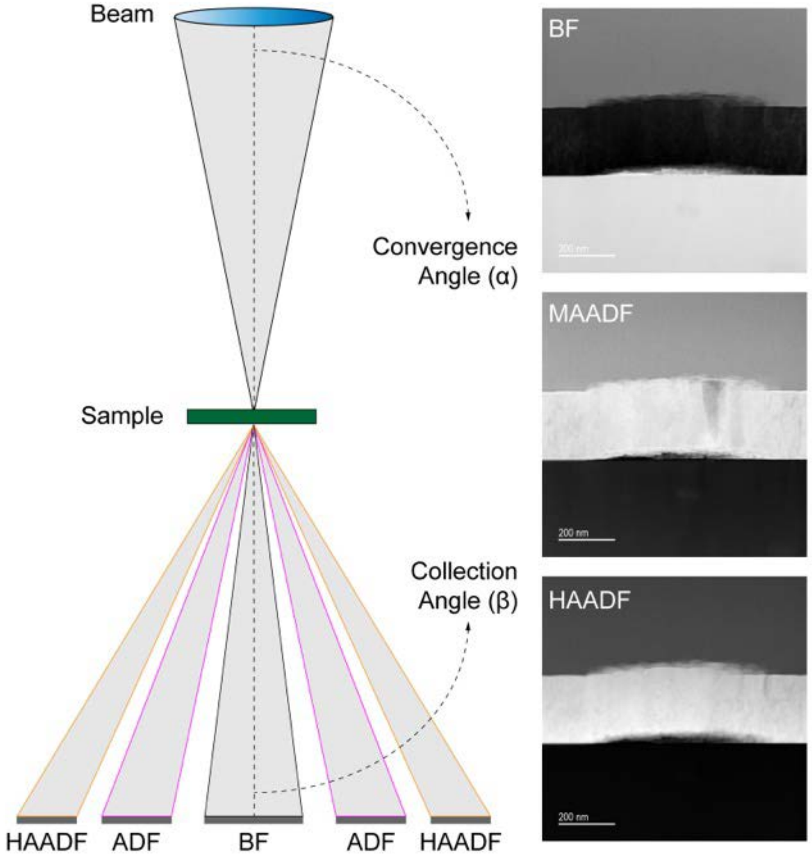


Spectroscopy

Du et al. Phys Rev B 2, 094602. (2018). | Popel et al. ACS Appl Mater Int. 12, 39781. (2020). | Spurgeon et al. PNAS 116, 17181. (2019).

The Challenge

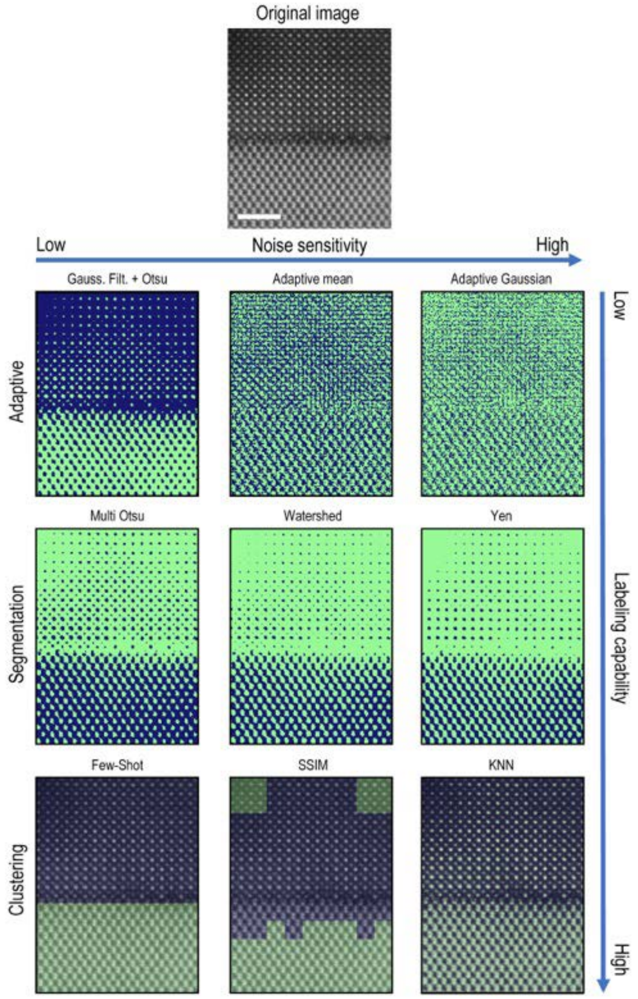
Imaging parameters strongly affect the representation of an object in data



Spurgeon. (2020). DOI:10.48550/arXiv.2001.00947

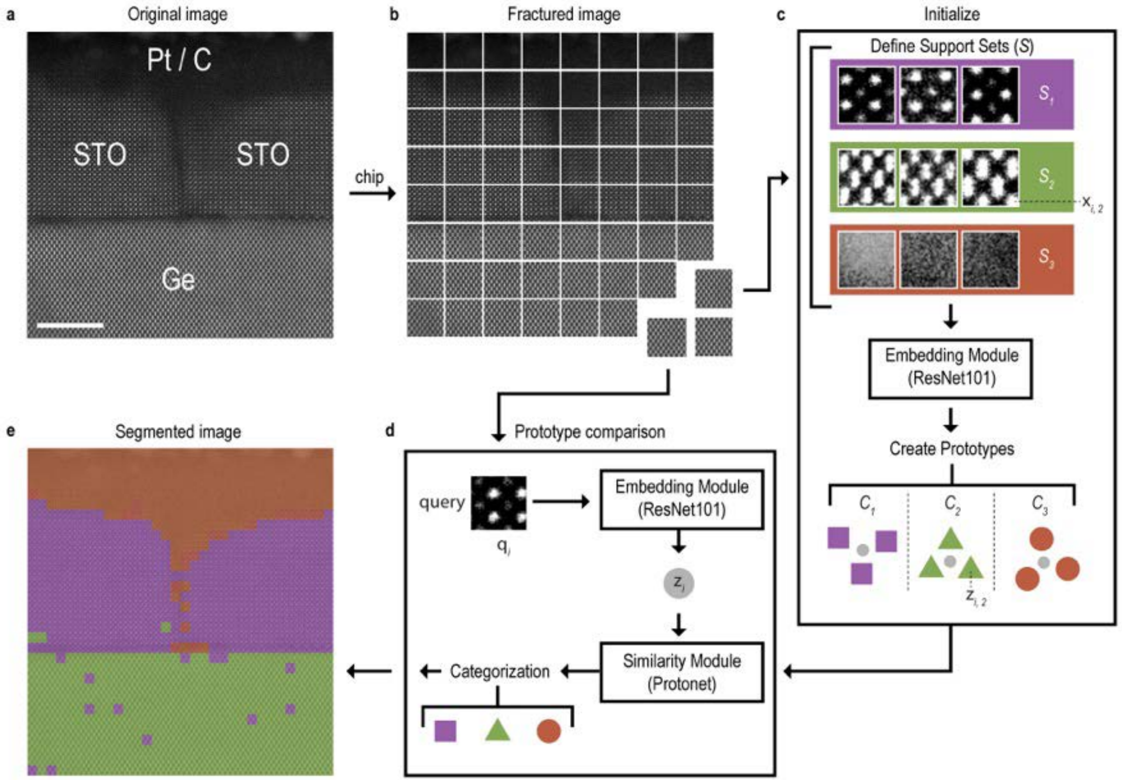
The Task

Classify microstructural features using limited examples



Akers et al. (2021). npj Computational Materials, 7(1), 187.

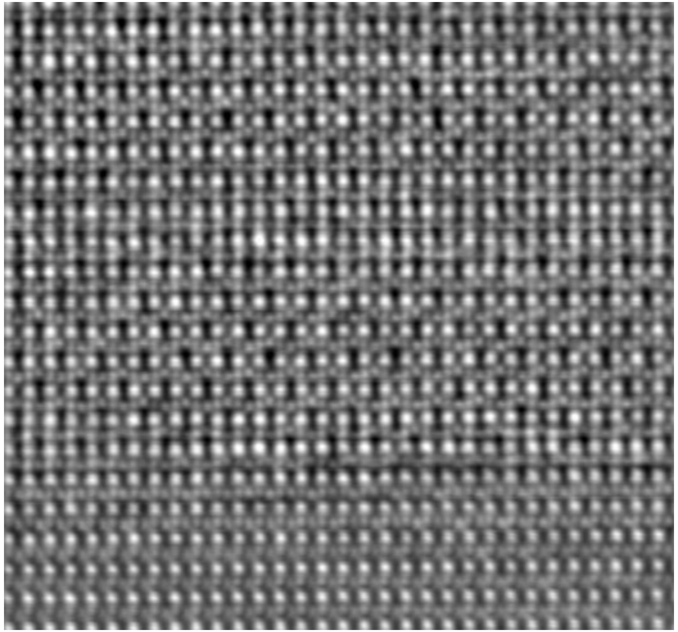
Few shot learning uses limited prior knowledge to classify features in discovery scenarios



Akers et al. (2021). npj Computational Materials, 7(1), 187.

Careful pre-processing is needed for best model performance

Without Contrast Leveling Adaptive Histogram Equalization (CLAHE)



2 nm

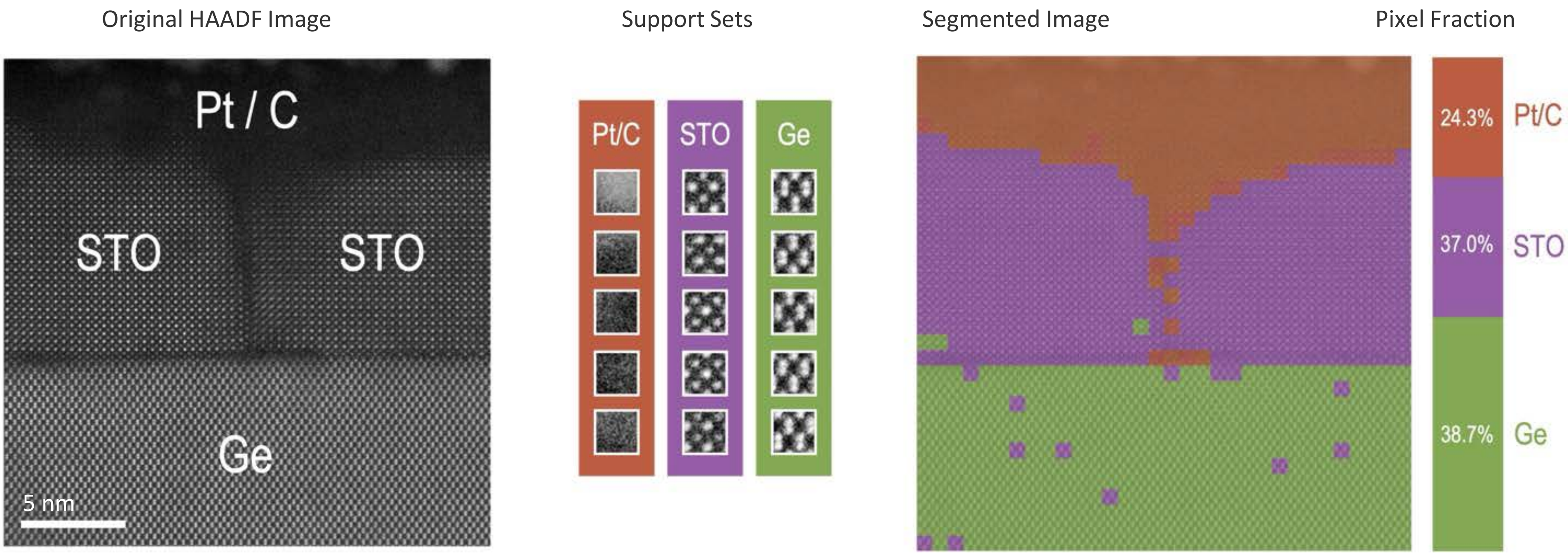
With CLAHE

Akers et al. (2021). npj Computational Materials, 7(1), 187.

A simple GUI can interact with model parameters and support sets for different tasks

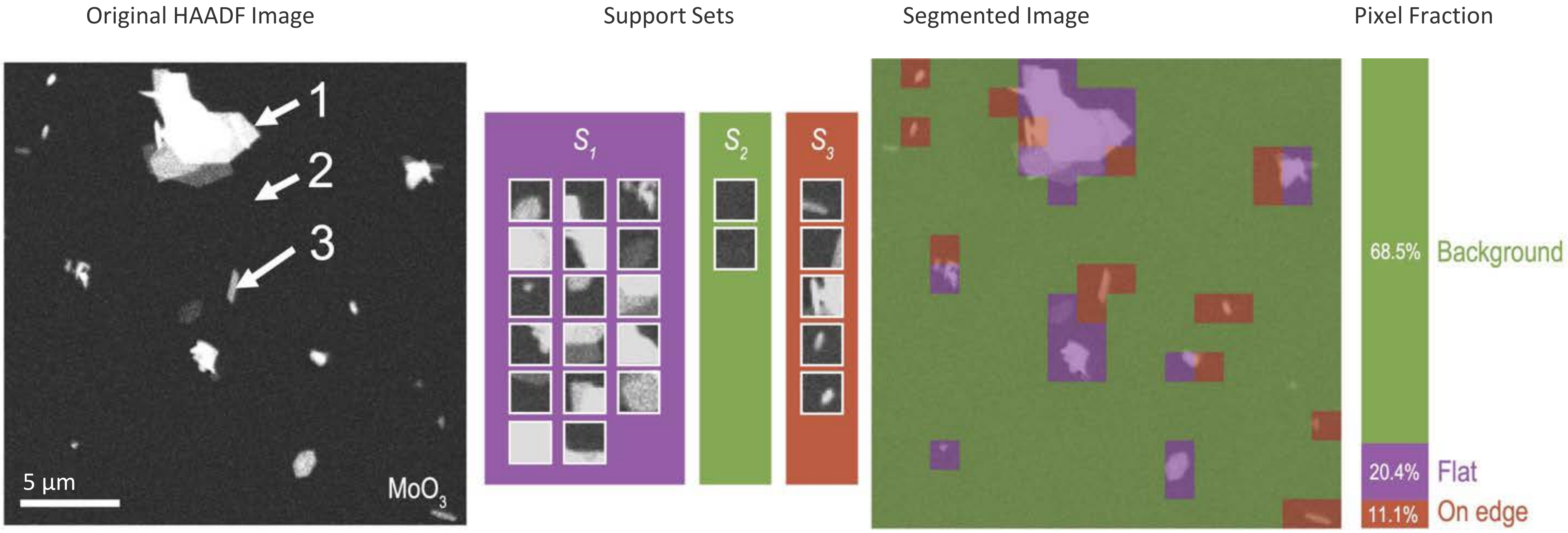
Doty et al. (2022). Computational Materials Science, 203, 111121.

We can rapidly classify atomic motifs in data to understand phase distributions



Akers et al. (2021). npj Computational Materials, 7(1), 187.

Such a model can easily be applied to different synthesis tasks

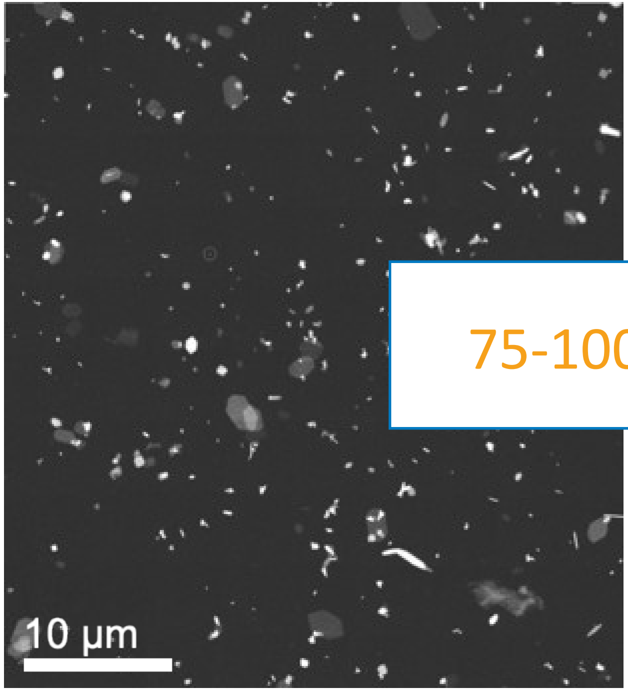


Akers et al. (2021). npj Computational Materials, 7(1), 187.

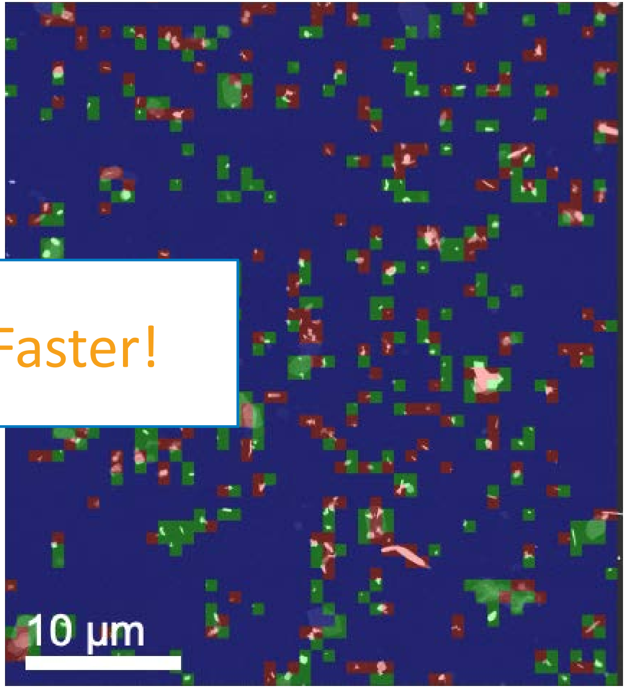
We can ultimately extract materials descriptors in a faster and more reproducible manner

MoO_3

Manual Analysis
10 minutes



75-100x Faster!

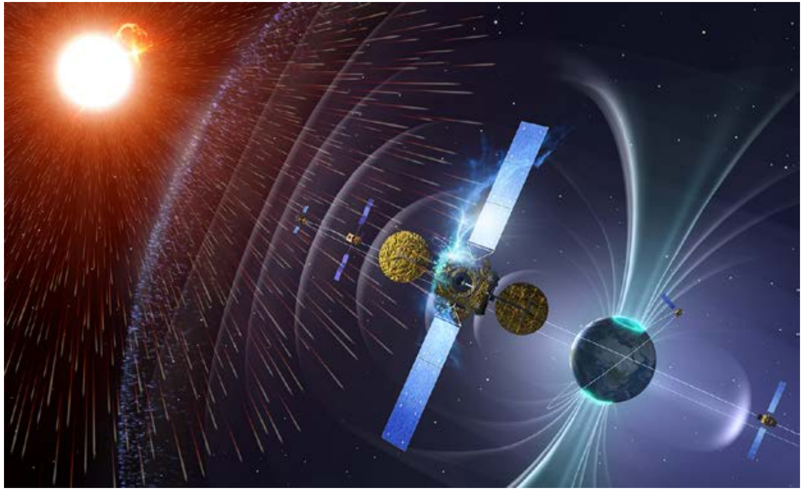


Few-Shot
Task 2
8 seconds

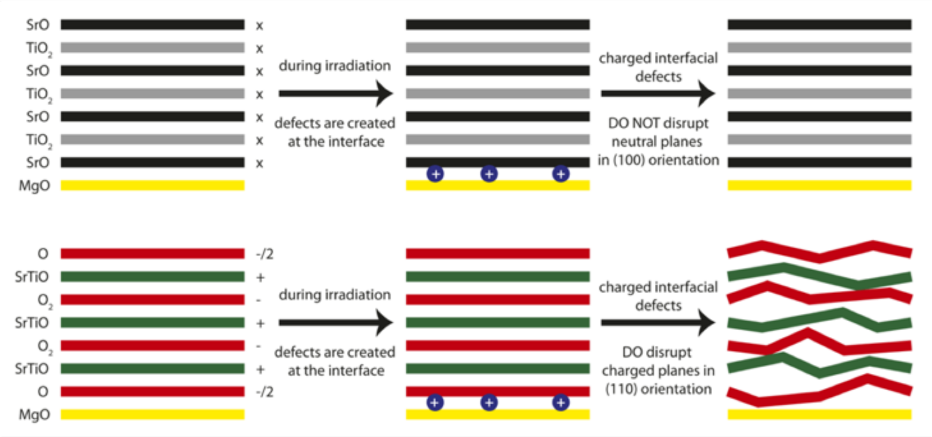
Doty et al. (2022). Computational Materials Science, 203, 111121. | Akers et al. (2021). npj Computational Materials, 7(1), 187.

Describing Disorder

Controlling materials degradation is critical for electronics and sensors in extremes

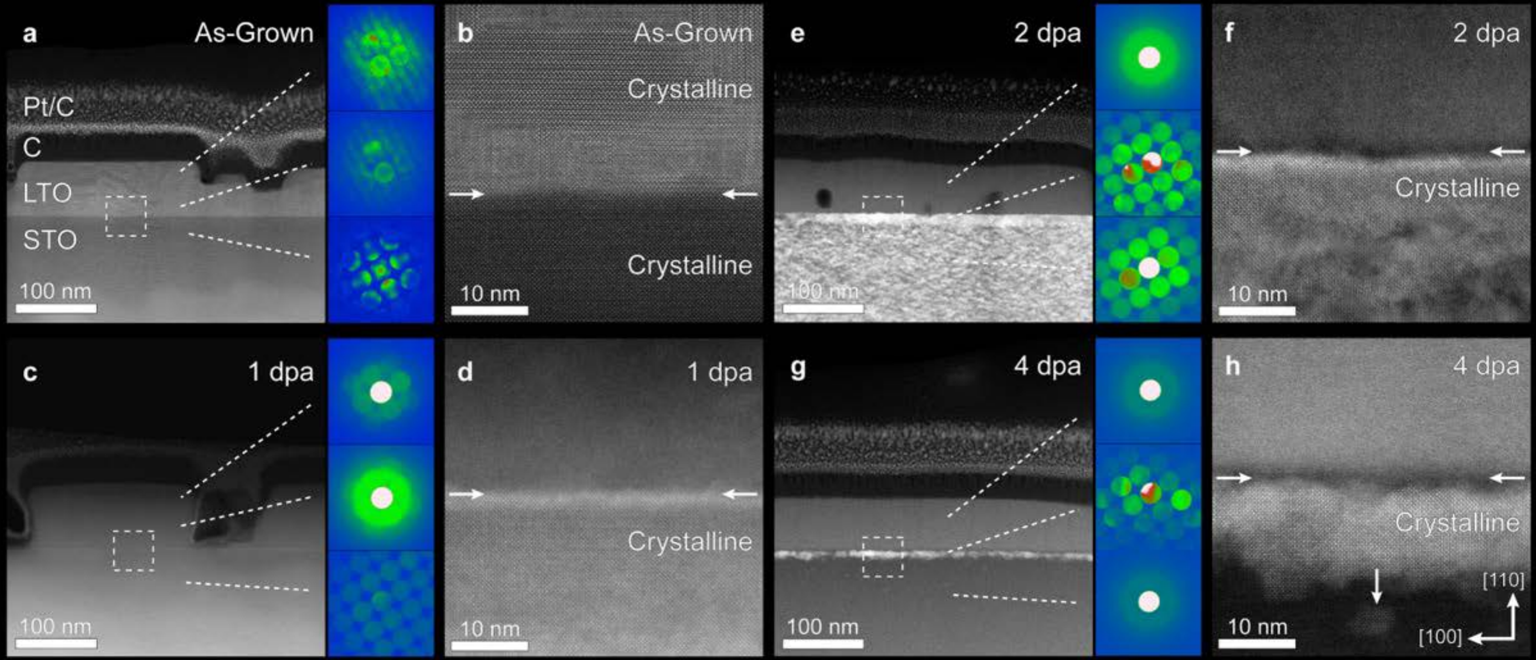


How does interface configuration affect radiation-induced disorder in devices?



Aguiar et al. J. Mater. Res. 29(16), 1699–1710 (2014). | Spurgeon. Curr. Opin. Solid. State Mater. Sci. 24(6), 100870 (2020). | Image: SSA / ESA

We can visualize damage buildup at these interfaces at stages of irradiation ex situ



Spurgeon, S. R. et al. Adv. Mater. Interfaces. 2020, 7(8). 1901901944.

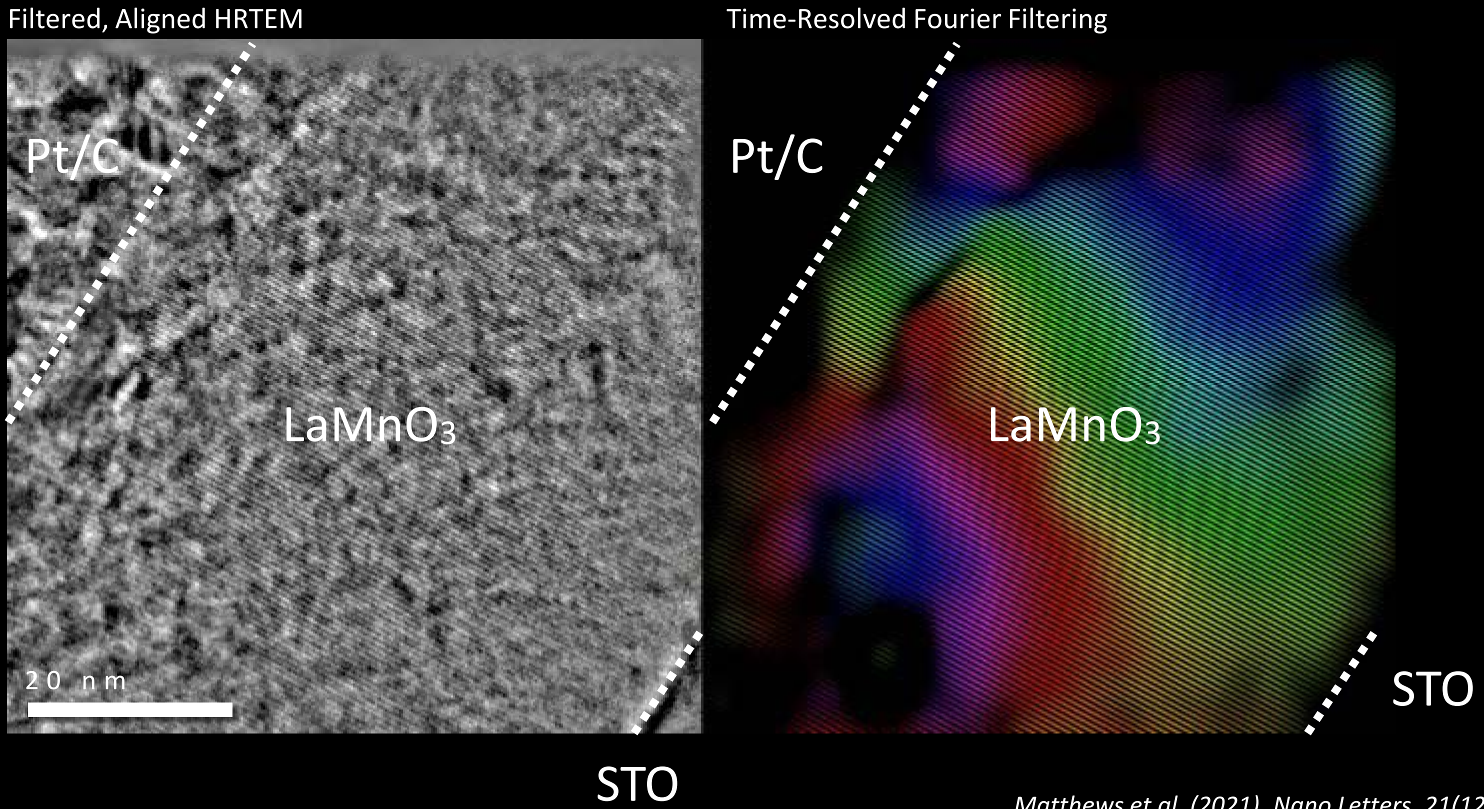
At CINT we took this one step further, visualizing materials breakdown in situ using the I³TEM

Khalid Hattar (UTK)

Chris Barr

https://tours.sandia.gov/ibl_info.html

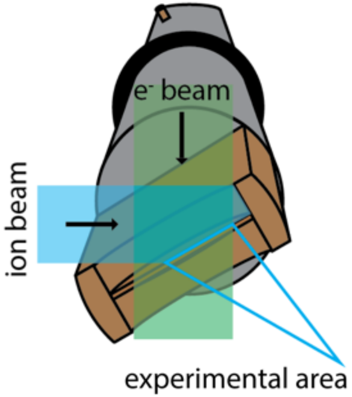
In situ TEM shows that disorder percolates through the material in a non-uniform manner

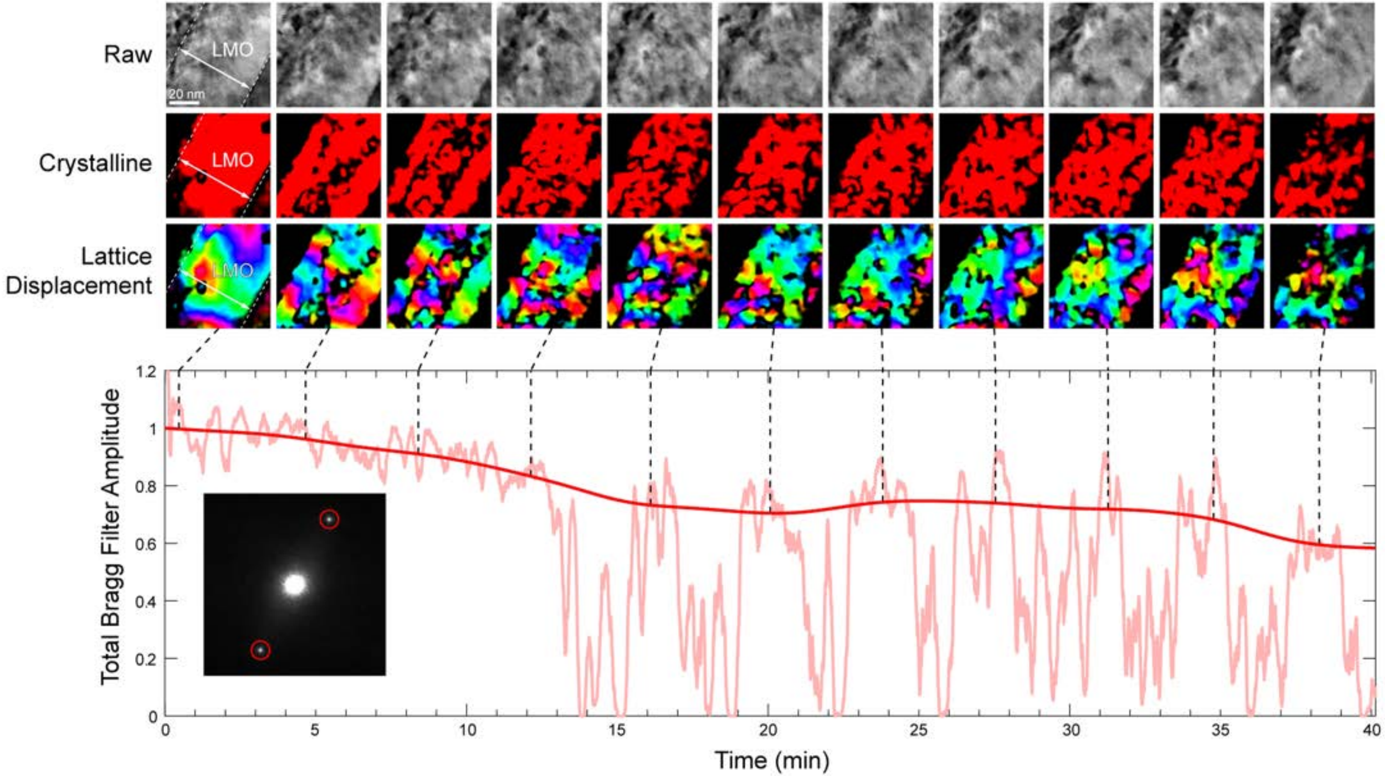


1 Hr Irradiation

Matthews et al. (2021). Nano Letters, 21(12), 5353–5359.

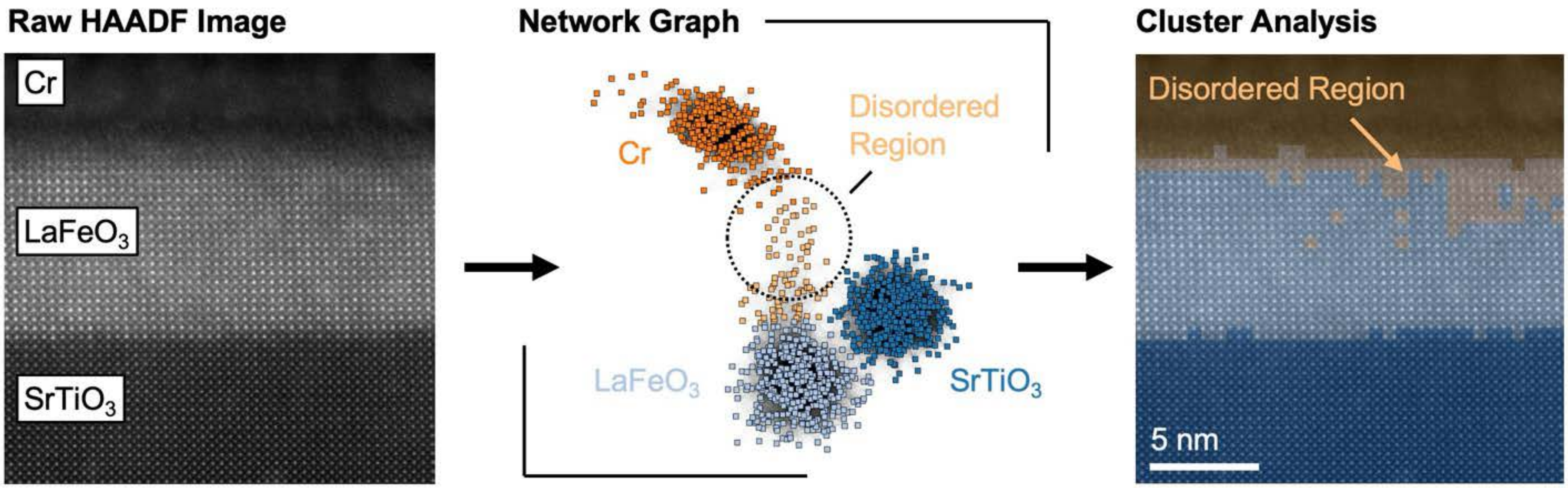
We can quantify the loss of crystallinity through statistical analysis of time series data





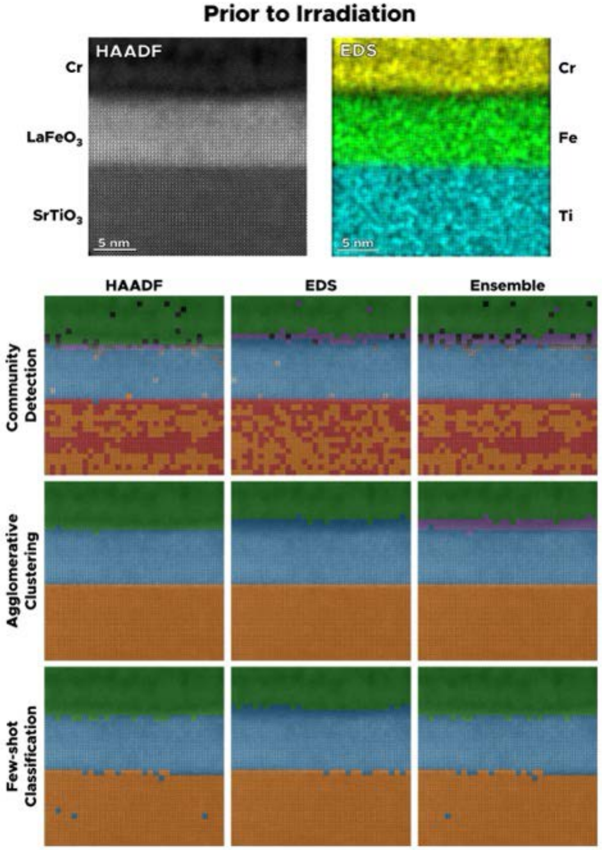
Matthews et al. (2021). Nano Letters, 21(12), 5353–5359.

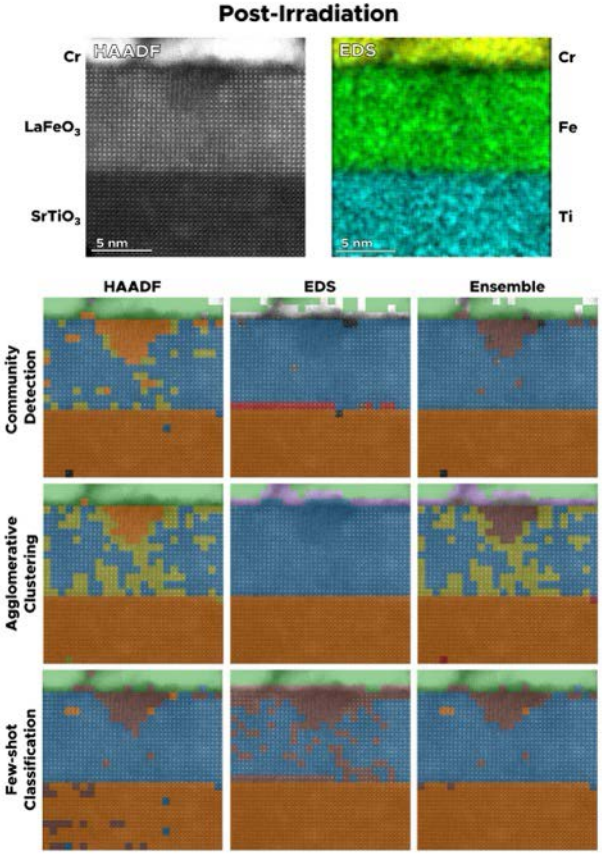
More recently, we have been developing unique order descriptors based on graph analytics



Ter-Petrosyan et al. Proc. Thirty-Seventh Conf. on Neural Information Processing Systems (NeurIPS). (2023). DOI:10.48550/arXiv.2311.08585

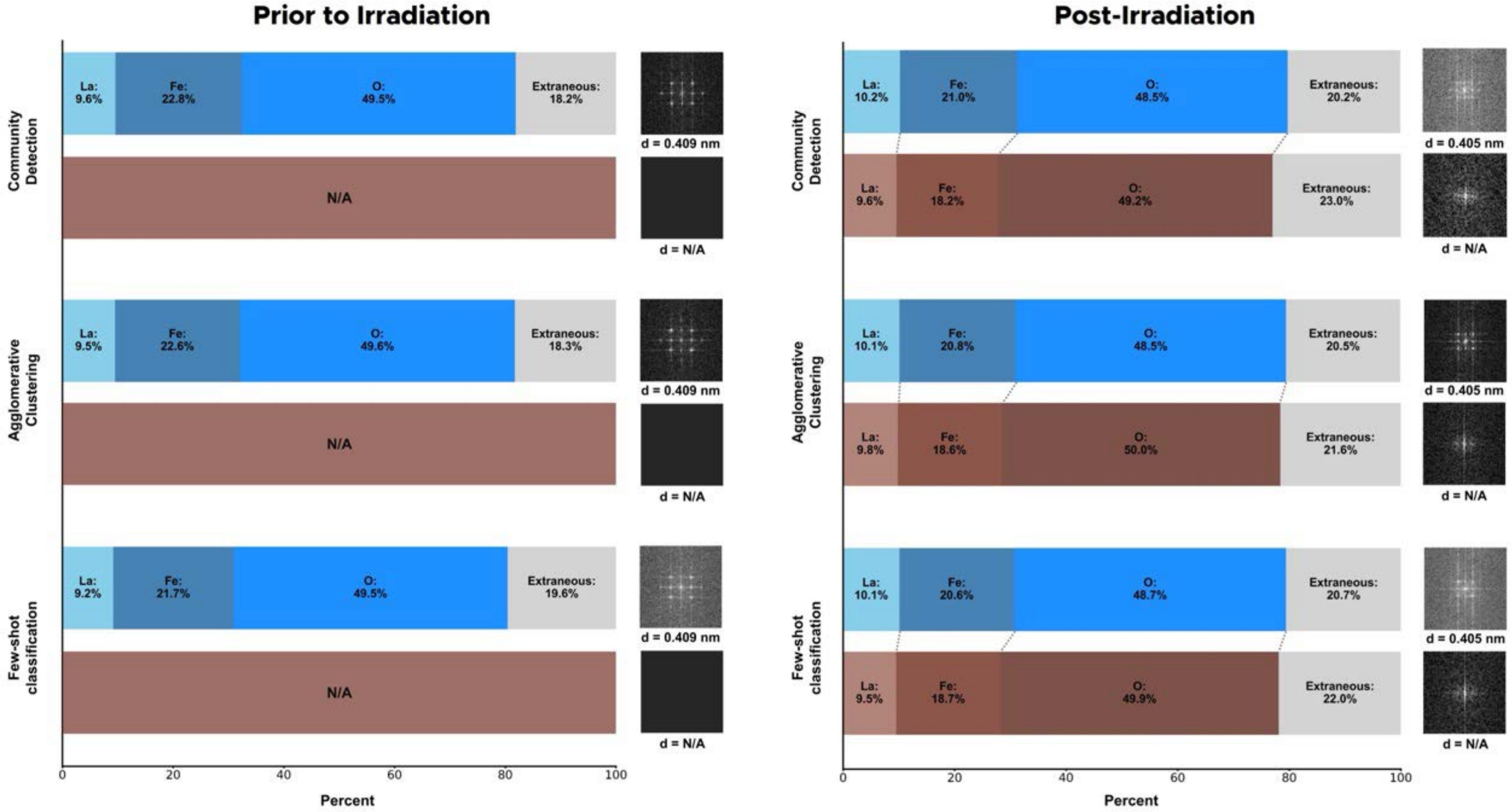
Multi-modal graphs effectively classify radiation damage signatures





Ter-Petrosyan et al. In preparation.

Such models reveal changes in composition associated with irradiation



Ter-Petrosyan et al. In preparation.

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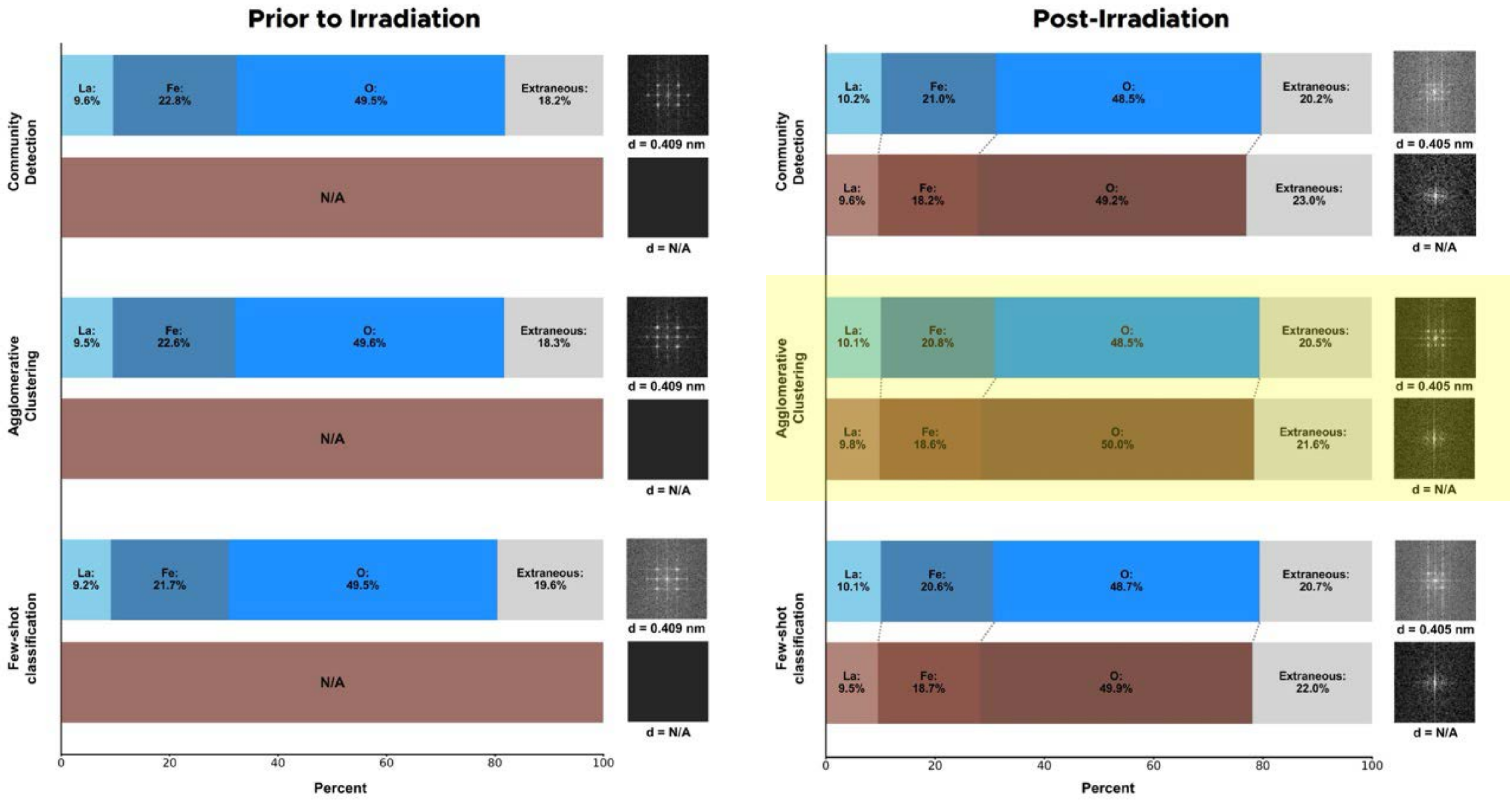
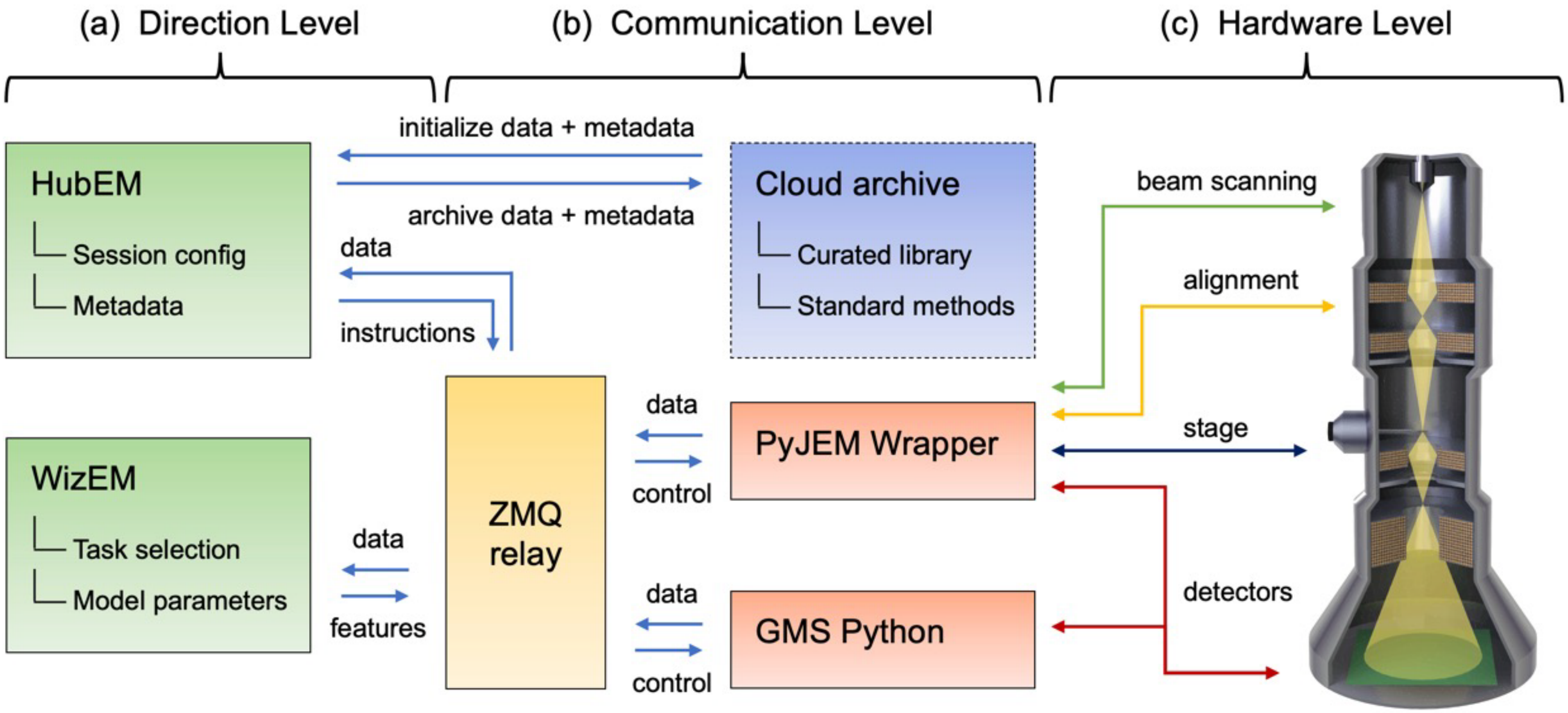


Ter-Petrosyan et al. In preparation.

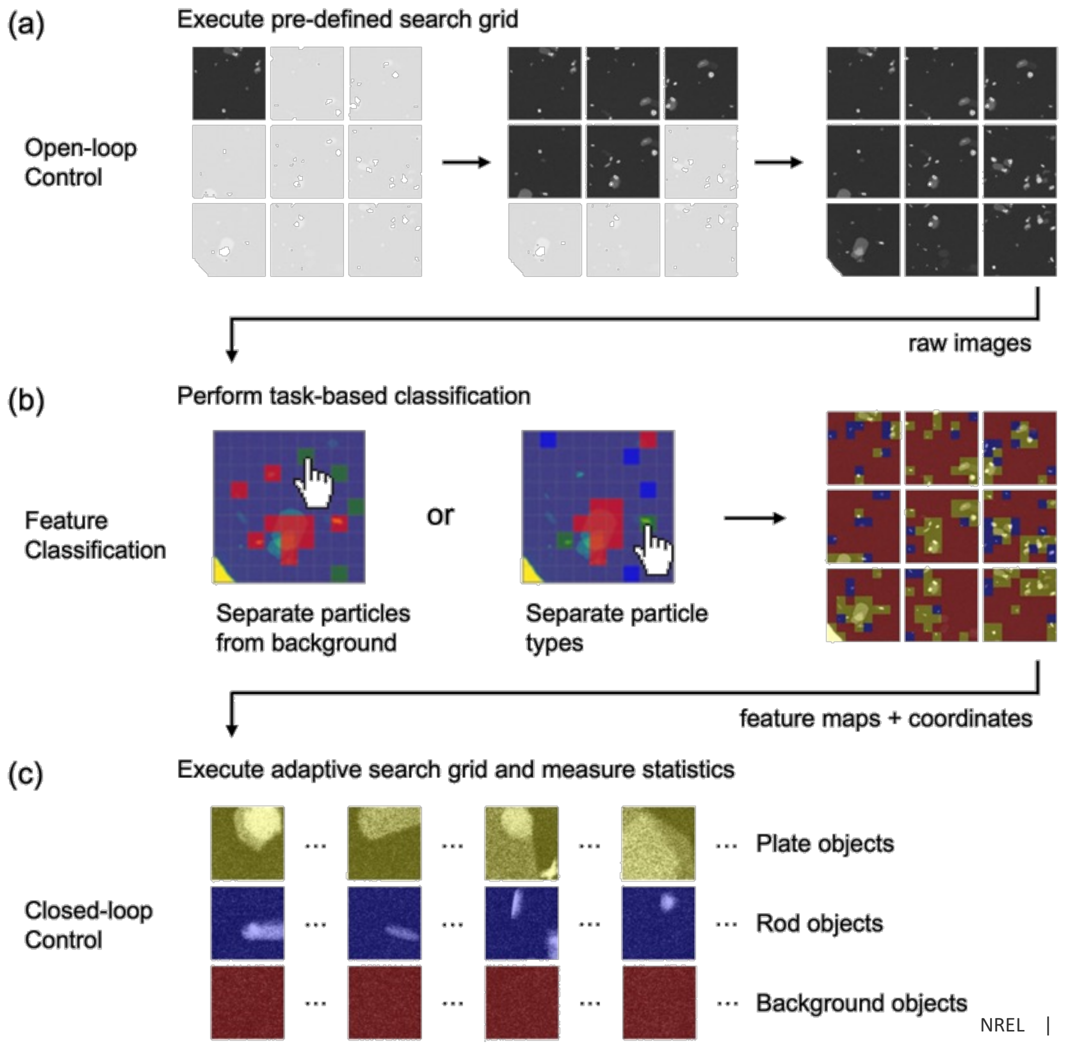
Toward Autonomous Experimentation

We have built an autonomous microscope platform based on few-shot and other ML models



Olszta et al. Microscopy and Microanalysis, 28 (5), 1611-1621. (2022).

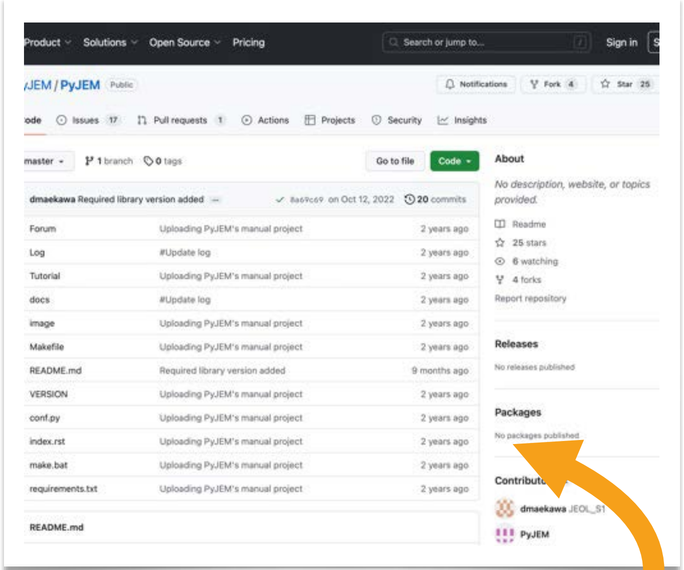
This platform enables intelligent closed-loop experiments and statistical analyses



Olszta et al. Microscopy and Microanalysis, 28 (5), 1611-1621. (2022).

PATENT PENDING
HTTPS://YOUTU.BE/XKYJ1UAE6JE

An Aside: Design of automated systems is challenging but it is getting easier

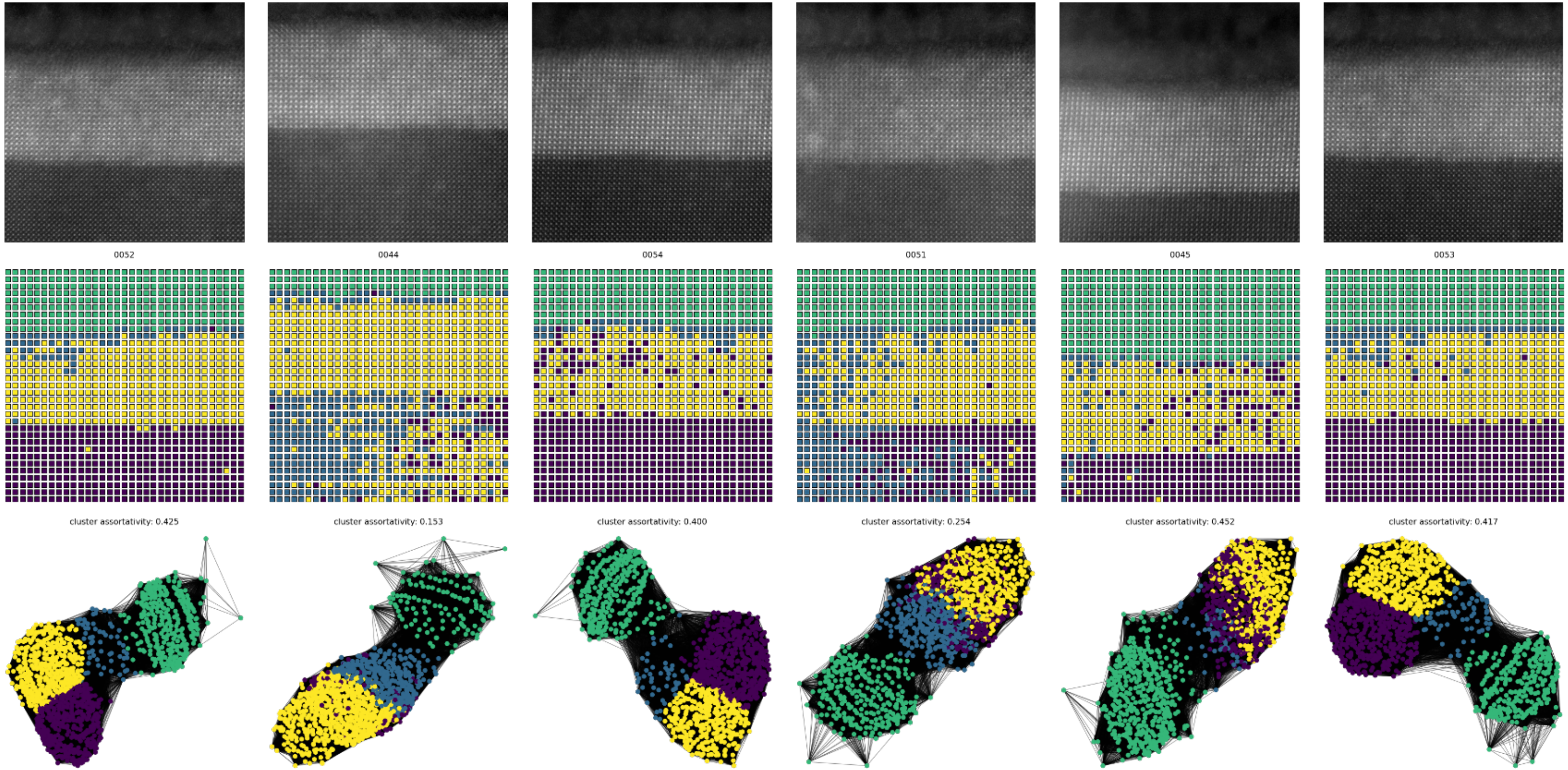


Get the PyJEM API!

- **Electronic optical system control** :
  Beam control, detector In / Out, magnification change, brightness change, etc..
- **Stage control** :
  Absolute position movement, Relative position movement, Piezoelectric movement, etc.
- **Image acquisition** :
  STEM or TEM image acquisition, image storage type change, resolution specification, etc.
- **Auto function** :
  Auto Focus, Auto Contrast Brightness, Auto Stigmator, etc.

https://github.com/PyJEM/PyJEM

We can build large libraries of synthesis and degradation pathways



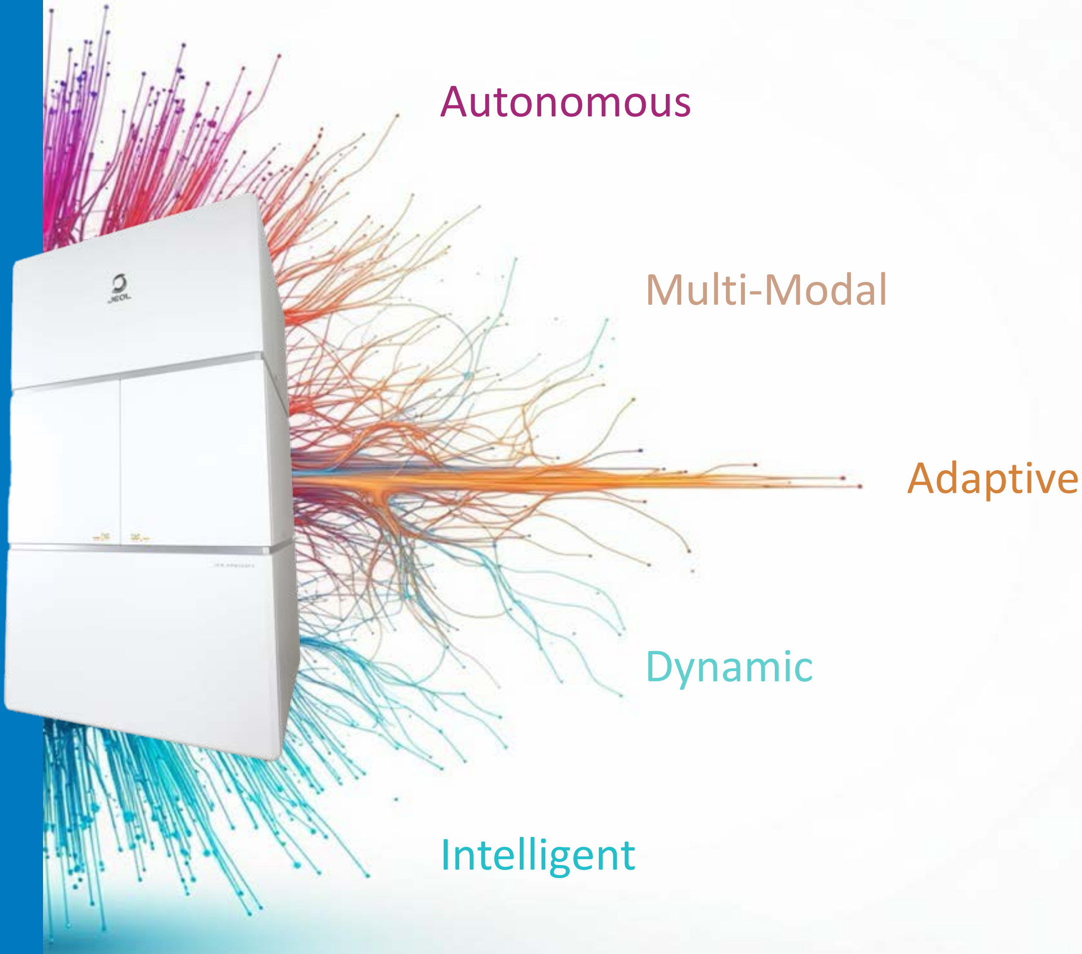
Ter-Petrosyan et al. Proc. Thirty-Seventh Conf. on Neural Information Processing Systems (NeurIPS). (2023). DOI:10.48550/arXiv.2311.08585

What is next?

NREL is leading a $14M recapitalization of our electron microscopy center, with a focus on in situ and autonomous science

What is next?

NREL will be home to a new autonomous electron microscope platform built around dynamic and adaptive experiments



AM^3

The Autonomous Multi-Modal Microscope

The Team

NREL

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Data Scientist

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PNNL

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Bethany Matthews
Materials Scientist

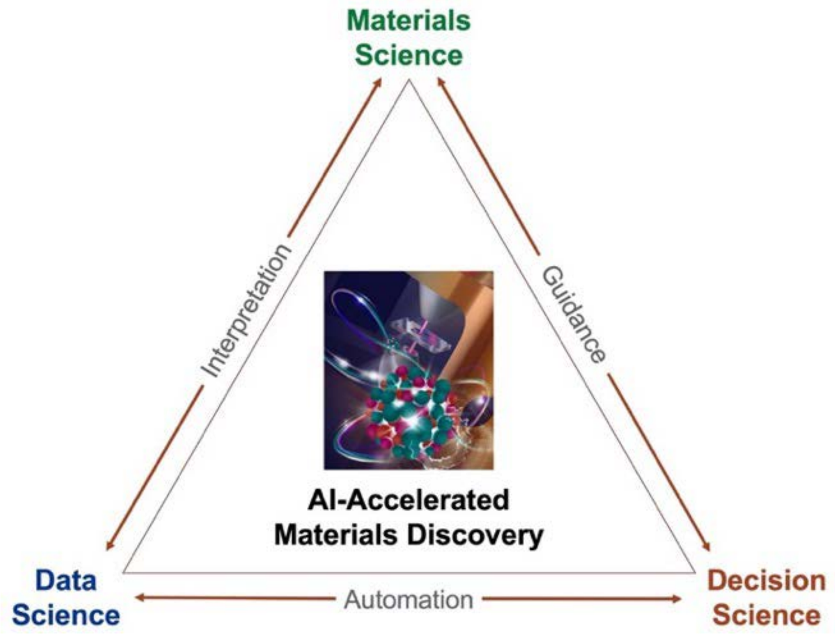
Tiffany Kaspar
Materials Scientist

Michel Sassi
Materials Scientist

Arman Ter-Petrosyan
Grad Student at UCI

Autonomous science is revealing previously hidden materials lifecycles and transforming the design of clean energy systems

For more information on electron microscopy @ NREL, visit: https://tinyurl.com/z8ryk4y3



NREL/PR-5K00-91894

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