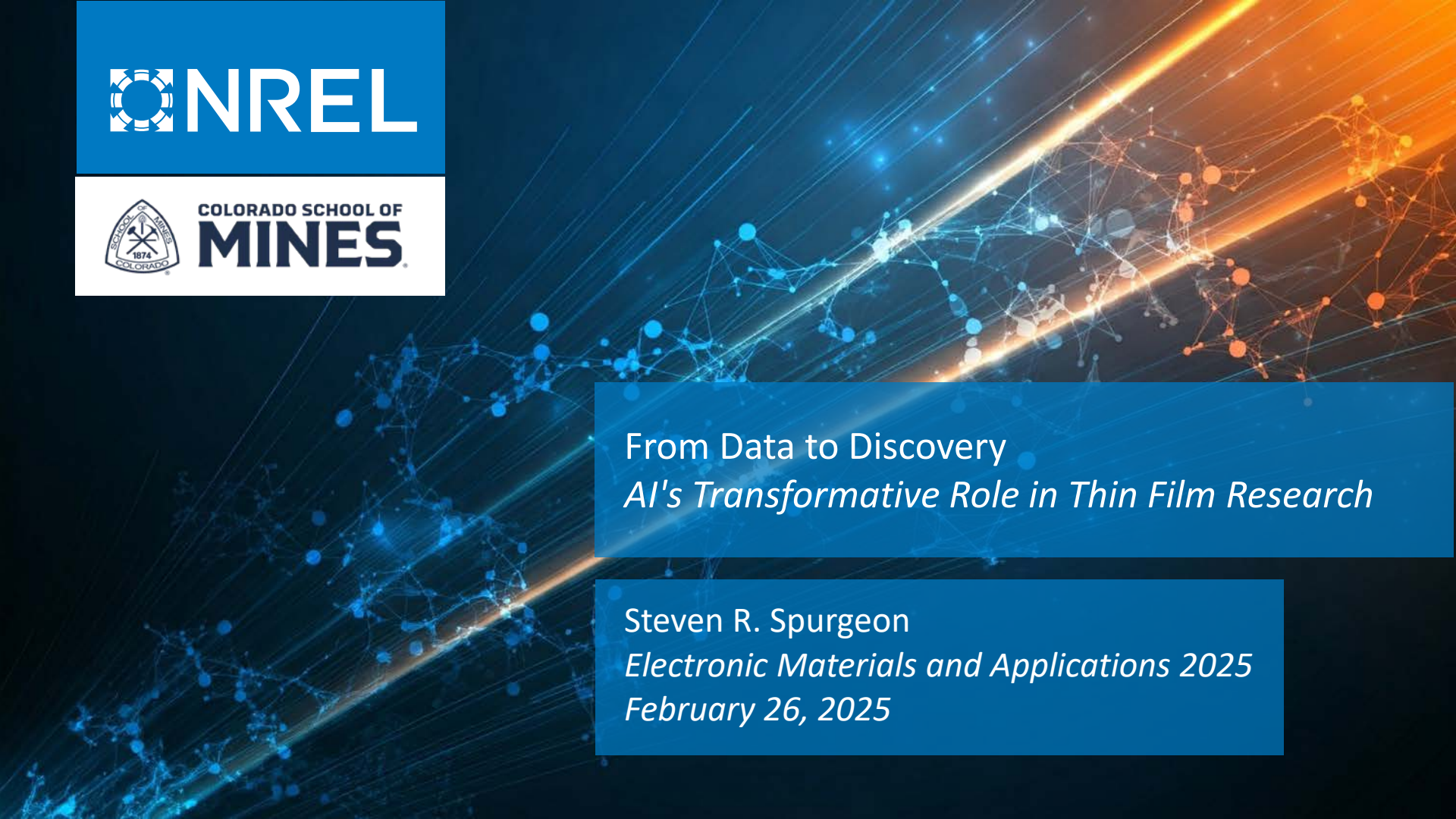
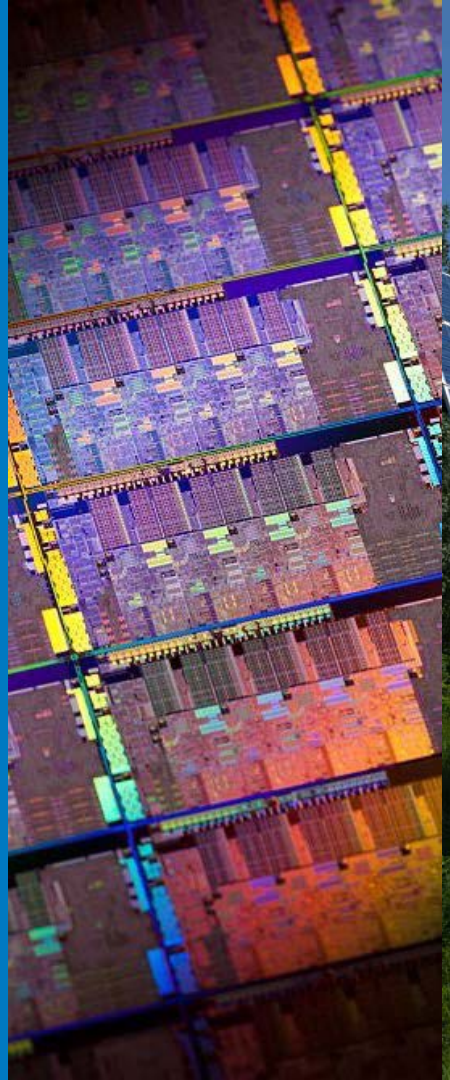
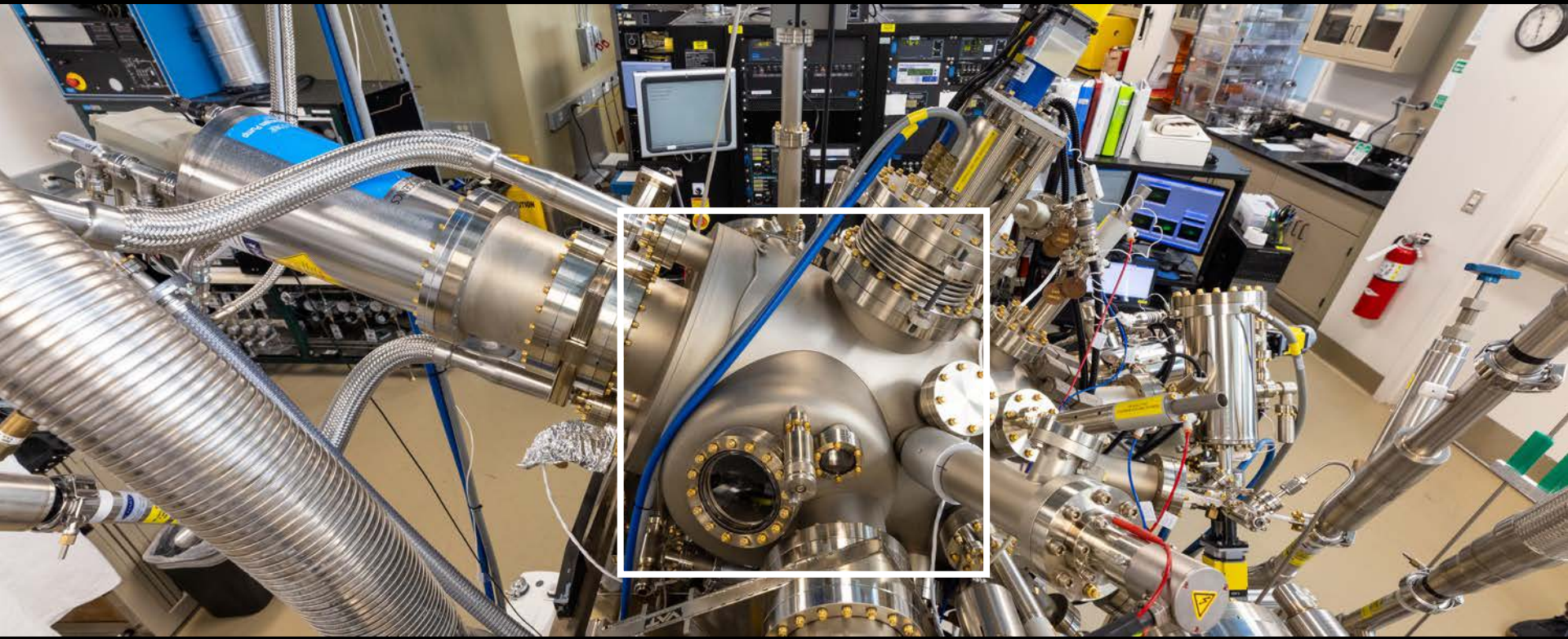

NREL
COLORADO SCHOOL OF
MINES
From Data to Discovery
AI's Transformative Role in Thin Film Research
Steven R. Spurgeon
Electronic Materials and Applications 2025
February 26, 2025

Everyday technologies are critically reliant on mastering materials lifecycles.



Wafer: Intel Company
PV: NREL
Battery: Battery Technology Online

Mastery depends on understanding of complex synthesis pathways…



CdTe MBE Lab @ NREL

Mastery depends on understanding of complex synthesis pathways…

Kaganer. Paul Drude Institute.

…and degradation behavior in real-world extreme environments.

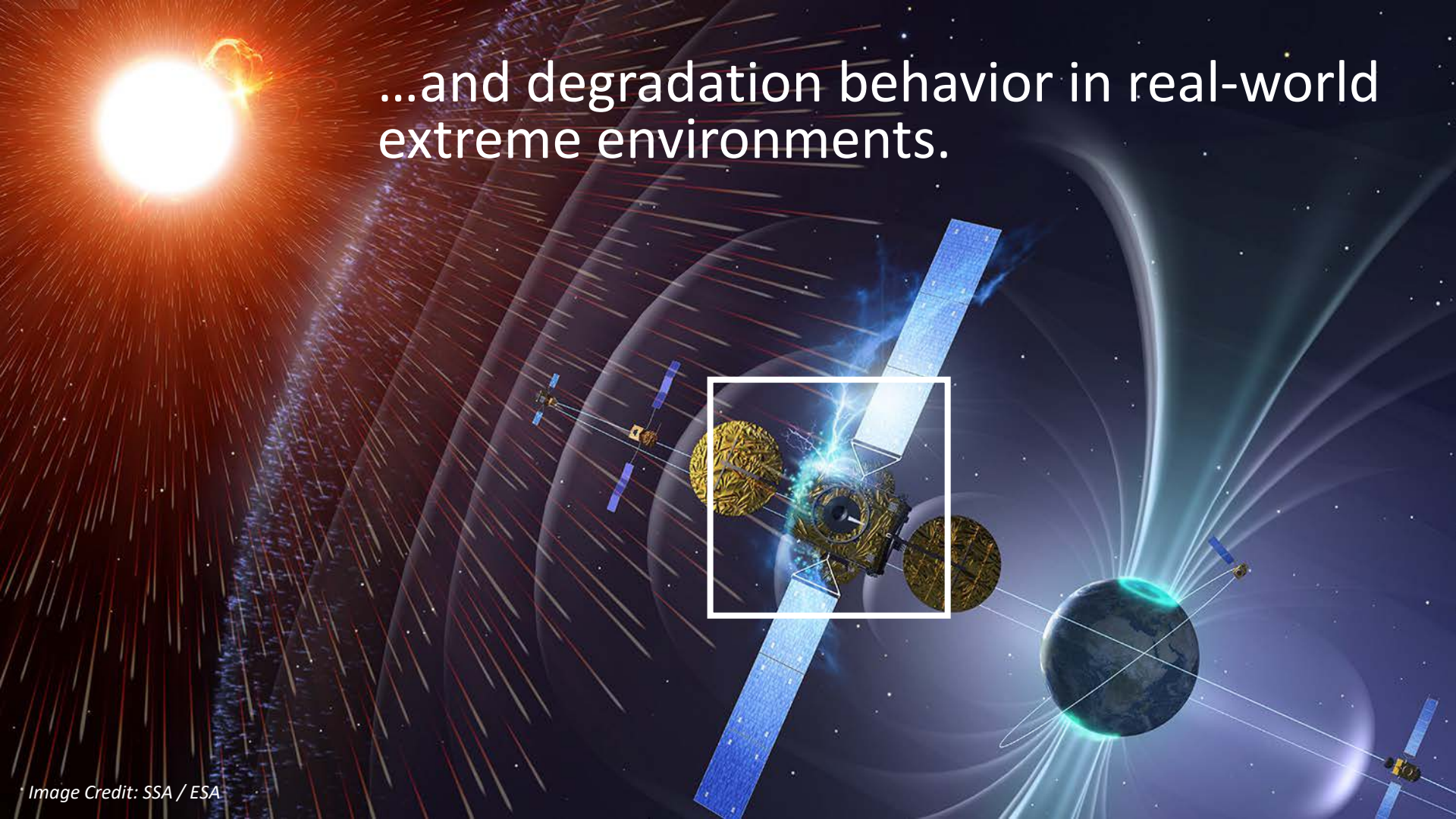
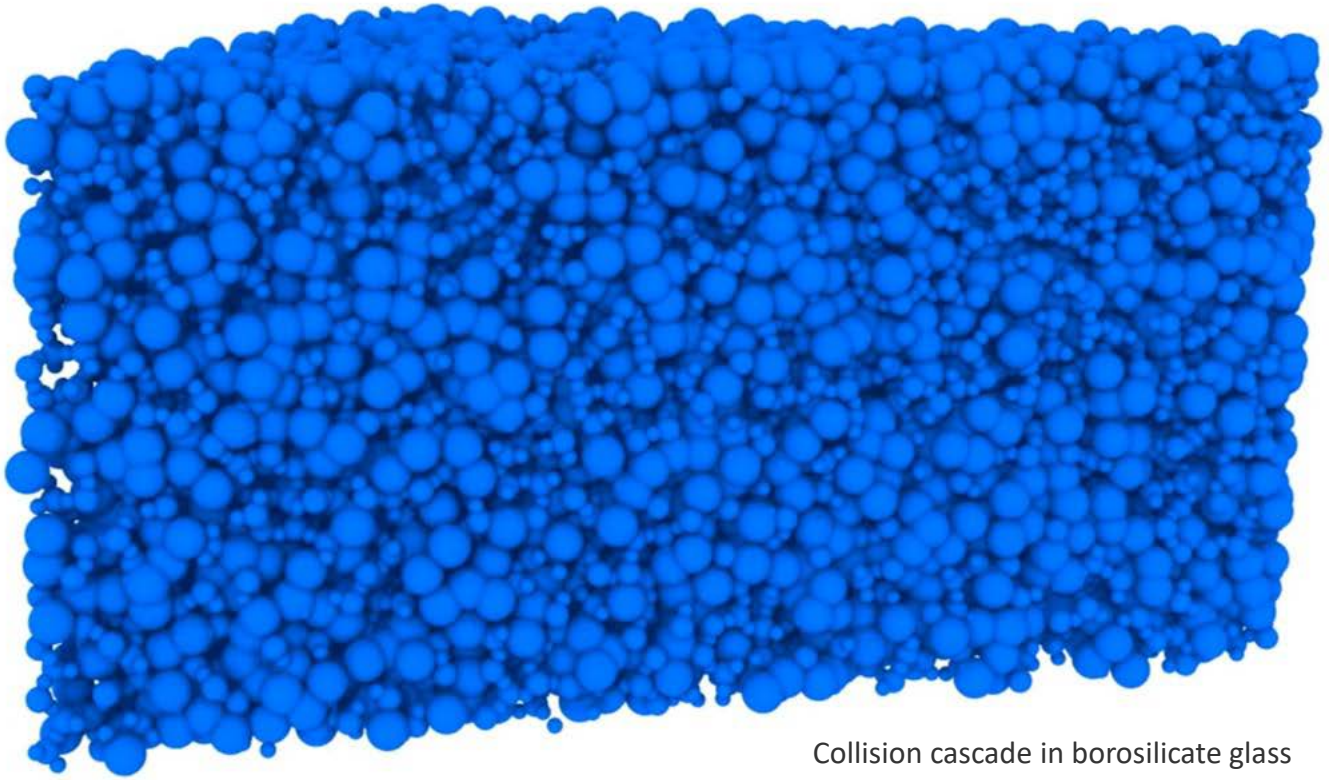


Image Credit: SSA / ESA

…and degradation behavior in real-world extreme environments.



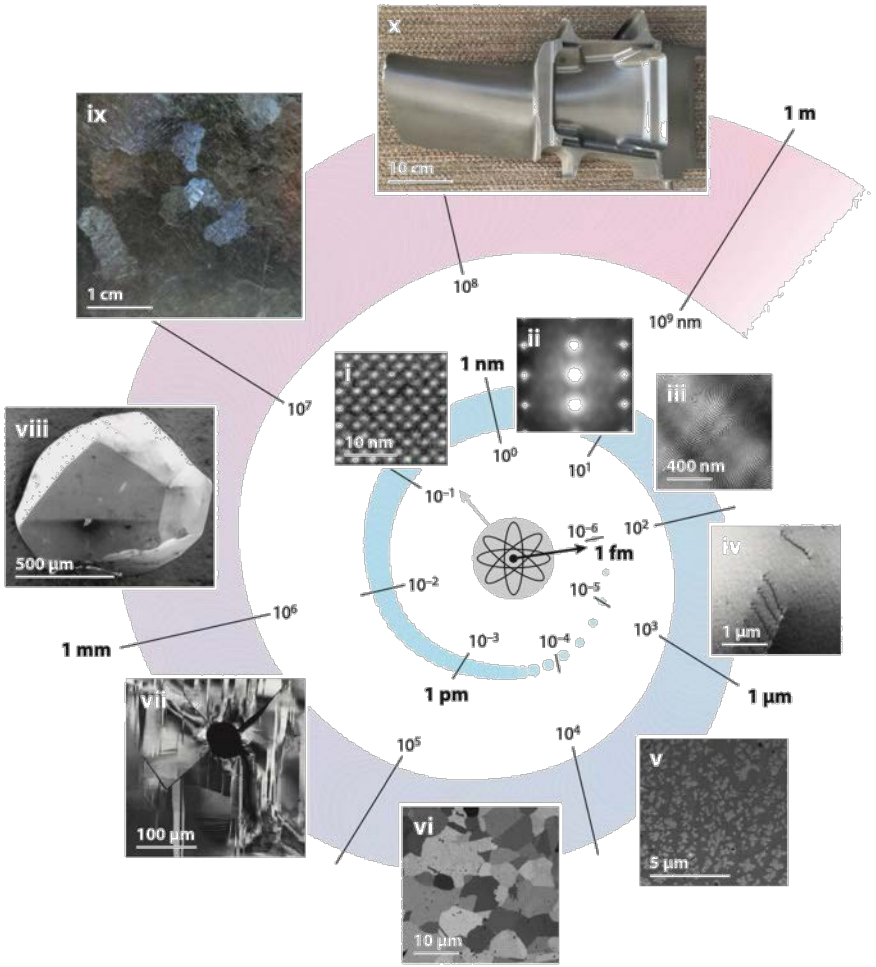
Collision cascade in borosilicate glass

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***

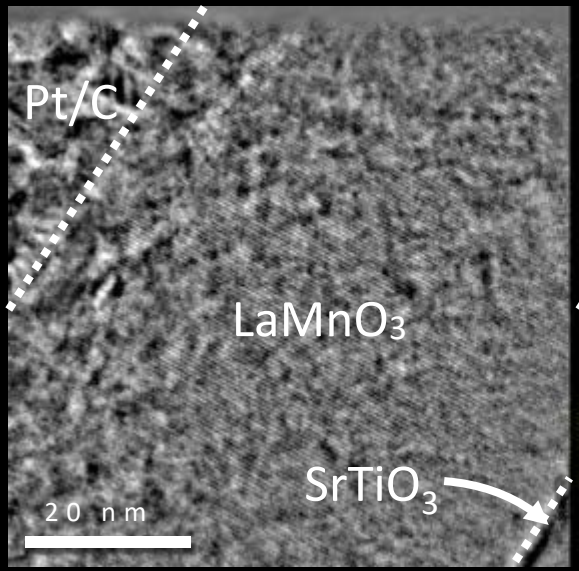
Quote adapted from: https://blog.palantir.com/ontology-finding-meaning-in-data-palantir-rfx-blog-series-1-399bd1a5971b



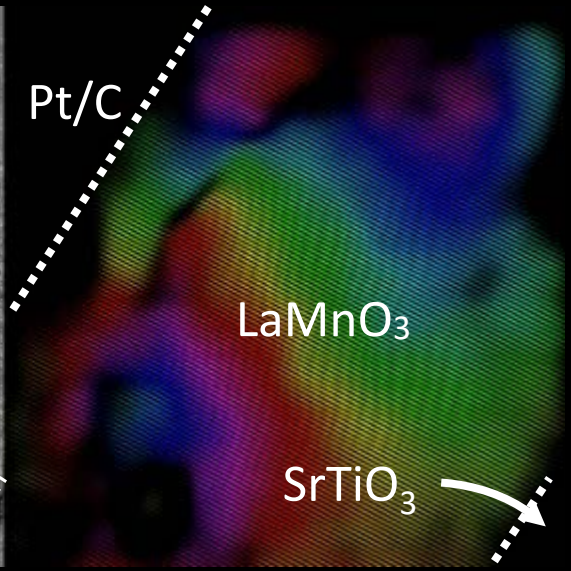
Kalidindi et al. Ann. Rev. Mater. Res. 45: 171-193. (2015).

We seek to understand how defects in functional thin films mediate disorder in extremes.

In Situ HRTEM During Irradiation



Time-Resolved Fourier Filtering

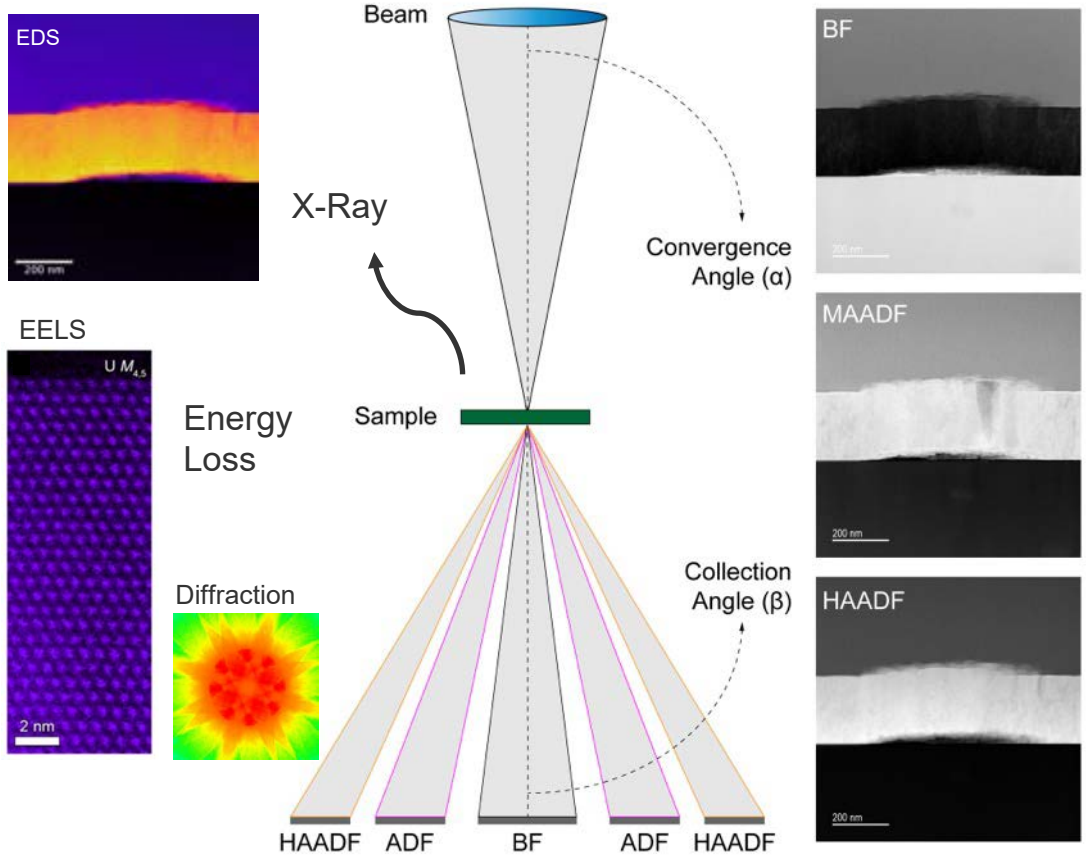


- What are the fundamental principles relating interface configuration and the response to radiation and other fields?
- Can we derive an order parameter that describes the disordering process enabling more robust design of thin film devices?

Image Credit: SSA / ESA

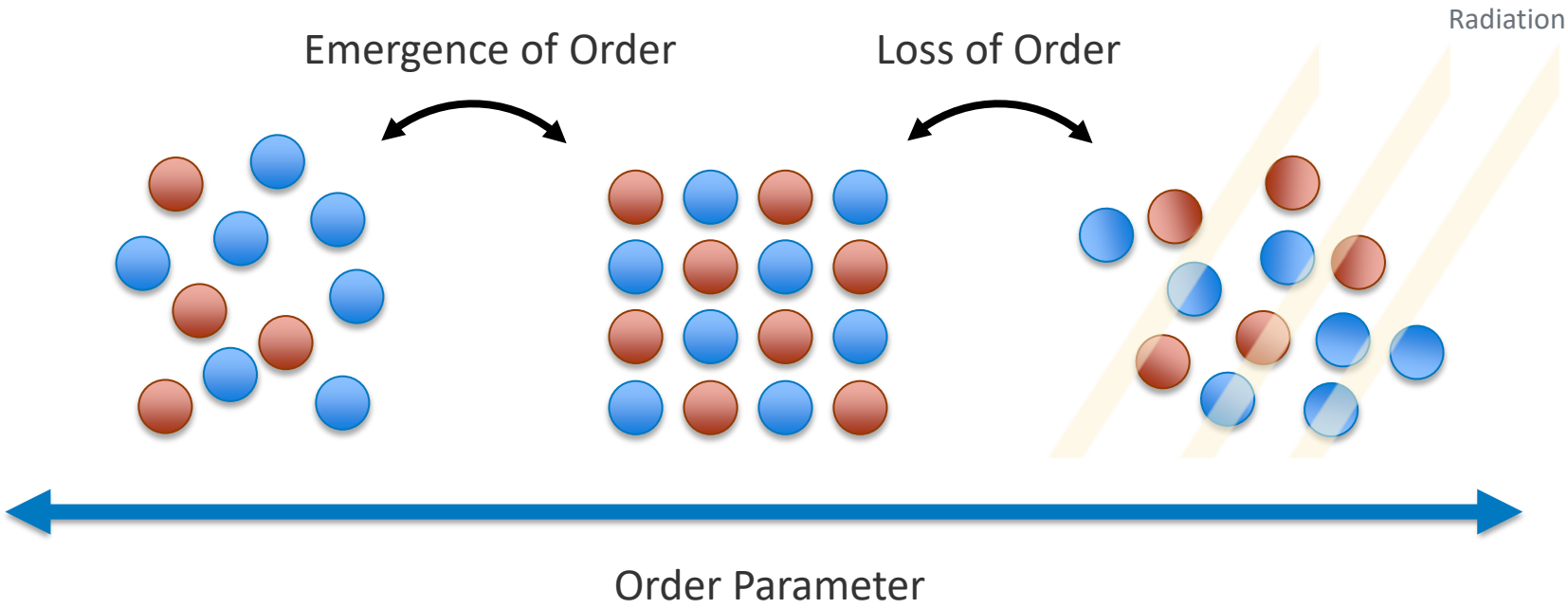
Matthews et al. Nano Letters, 21(12), 5353–5359. (2021).

The Challenge
How do we move from laborious one-off “hero” microscopy to truly statistical models?

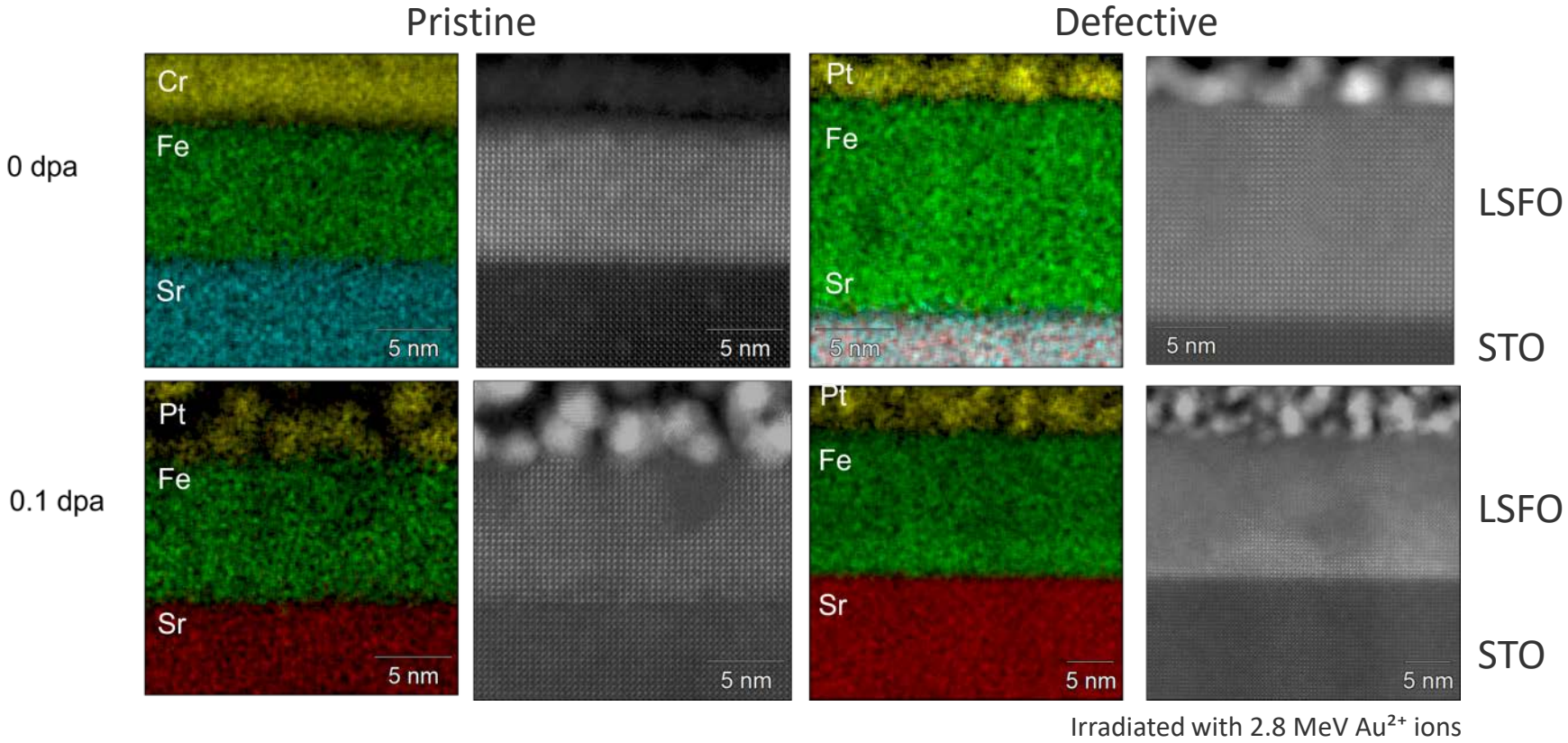


Spurgeon. (2020). DOI:10.48550/arXiv.2001.00947
Spurgeon et al. PNAS 116, 17181. (2019).

And can ML models inform an order parameter for the evolution of crystalline materials?



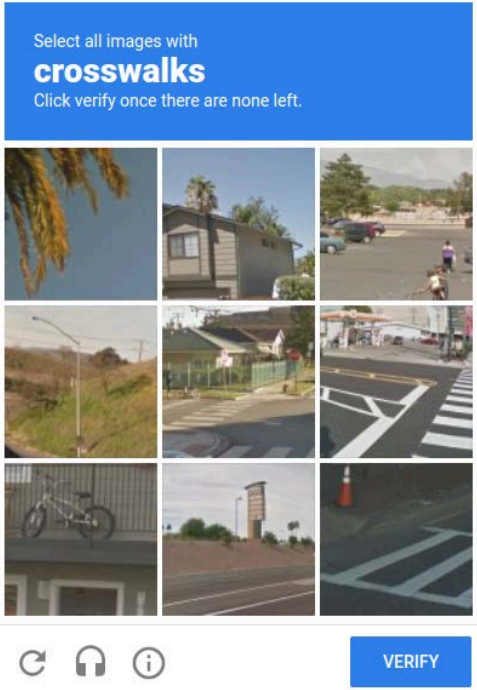
We examine the effect of initial microstructure and vacancy content on disordering pathways in $La_{1-x}Sr_xFeO_3$.



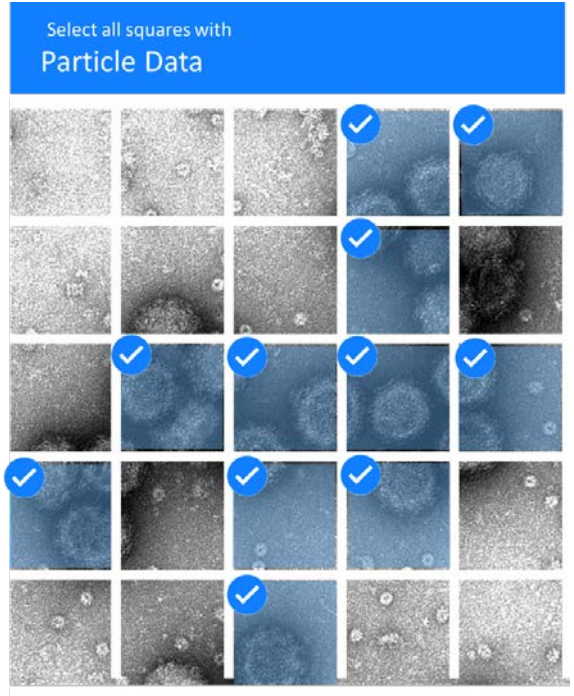
Ter-Petrosyan, A. et al. arXiv (2024). 10.48550/arXiv.2411.09896

Back in 2019, we considered possible ML-based solutions to handling our “sparse data” problem.

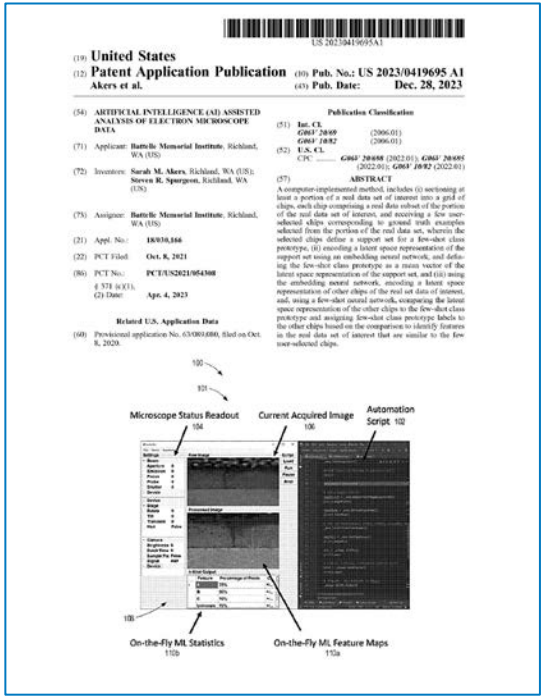
Google CAPTCHA Security



Few-Shot Learning for EM

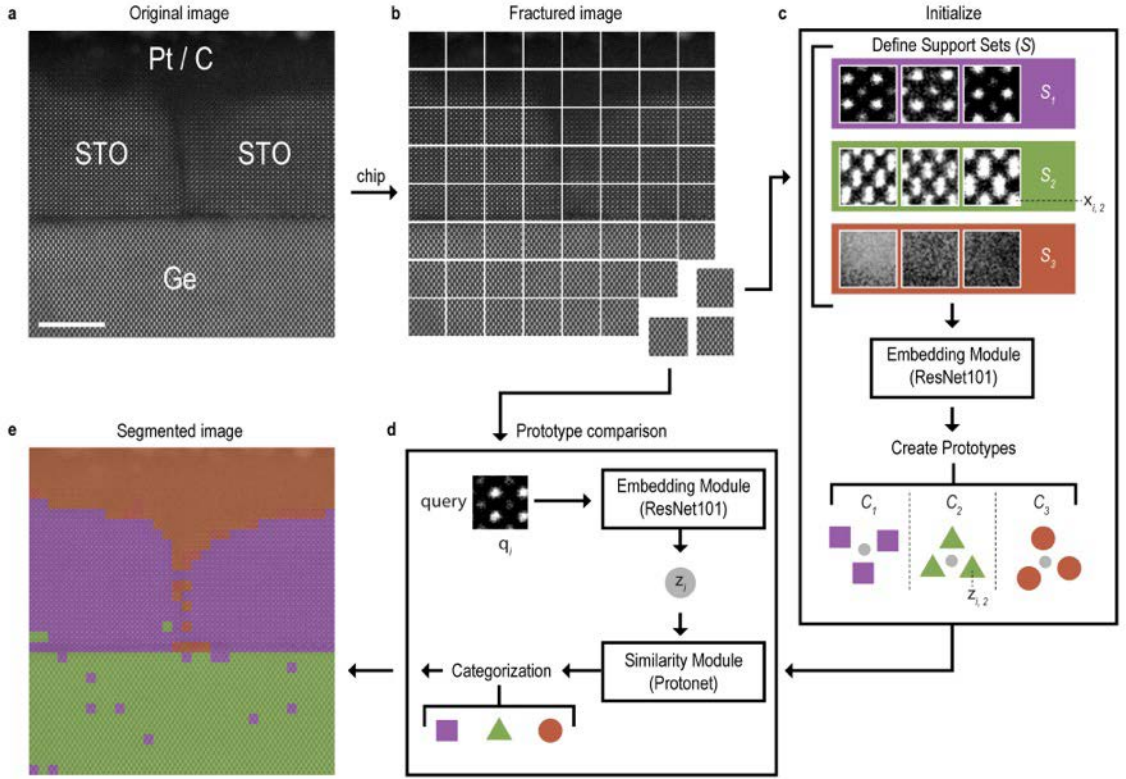


AI Microscopy Technology



https://patents.google.com/patent/US20230419695A1/en

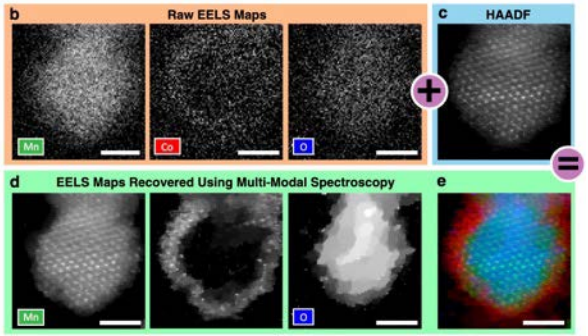
Few shot ML uses limited prior knowledge to classify features in discovery scenarios.



Akers et al. npj Comp. Mater., 7(1), 187. (2021).

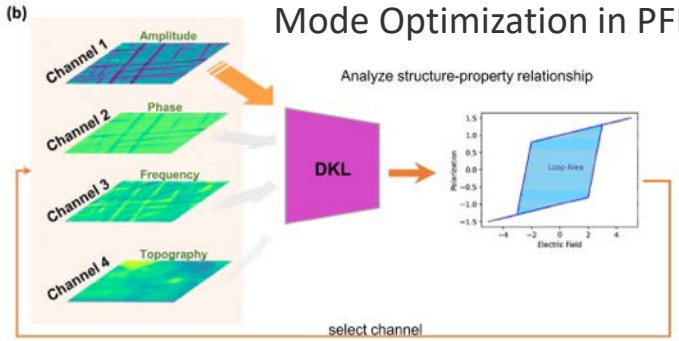
Multi-modal models provide a potentially powerful window into the materials lifecycle.

Fused Multi-Modal STEM



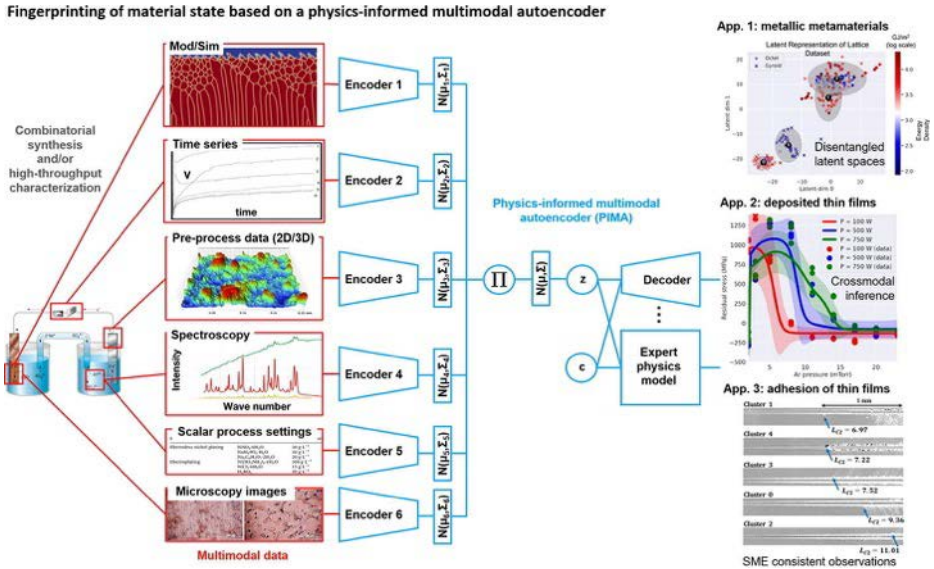
Schwartz et al. npj Comp. Mater. 8, 16 (2022).

Mode Optimization in PFM



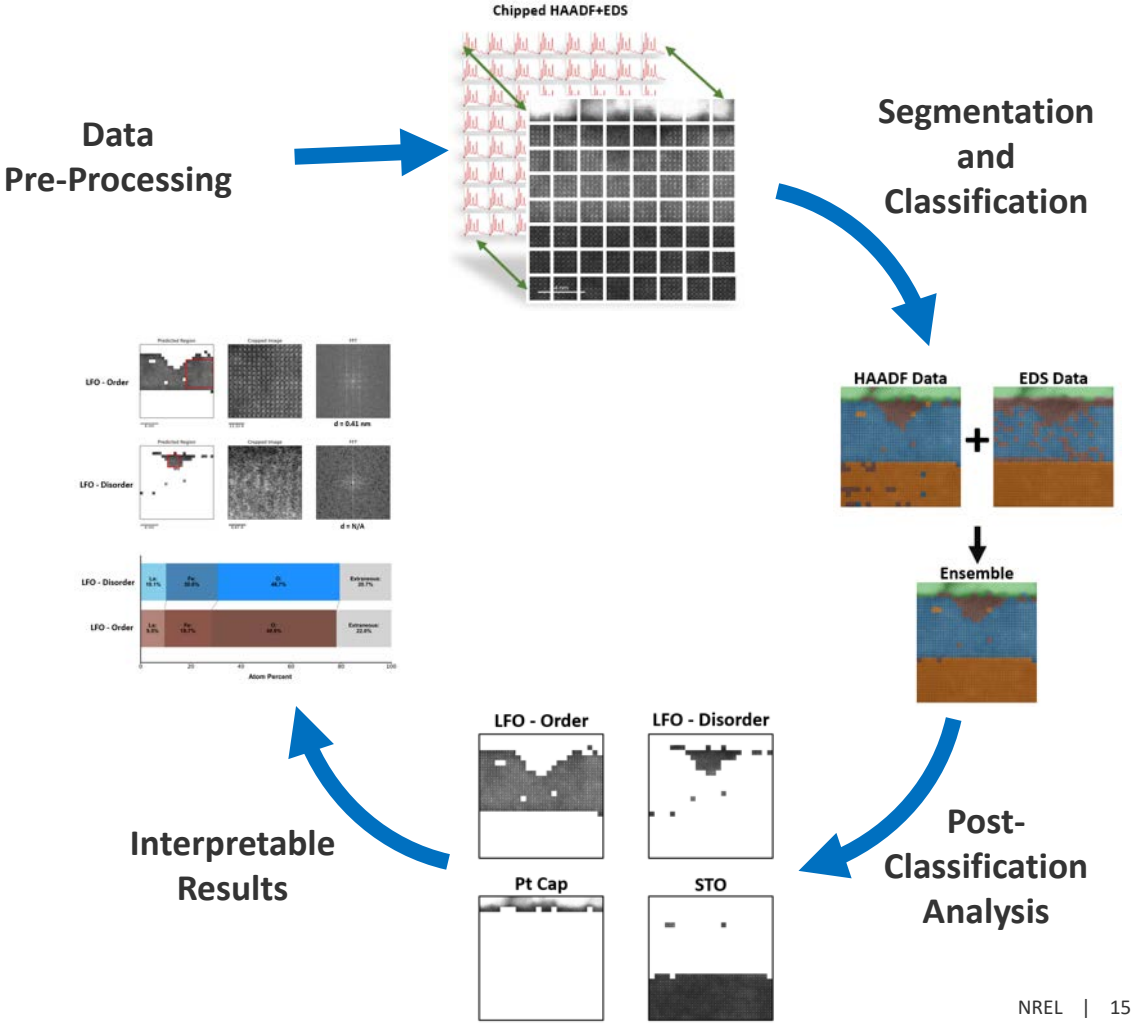
Liu et al. npj Comput. Mater. 9, 34 (2023).

Multi-Modal Autoencoders for Materials



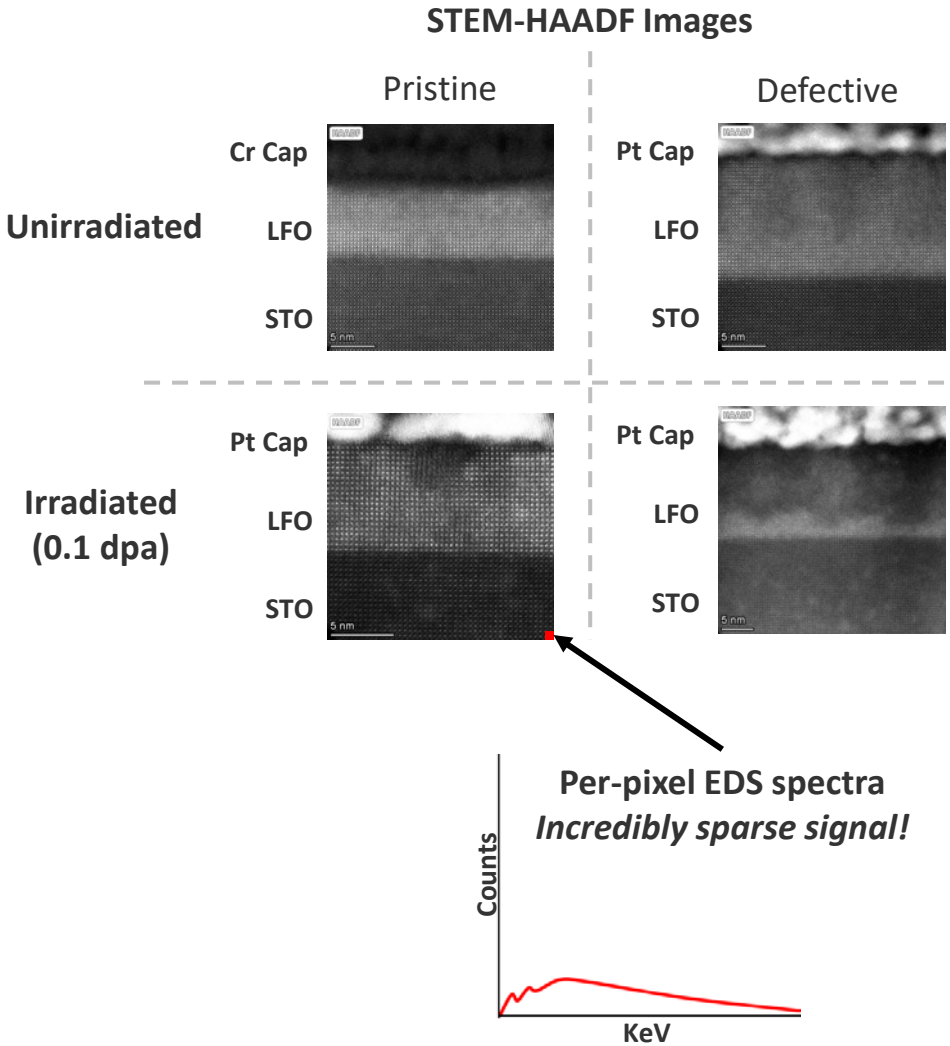
Trask et al. Mater. Today. 80, 286 (2024).

Our goal is to design a multimodal model that can incorporate both imaging and spectroscopy data.



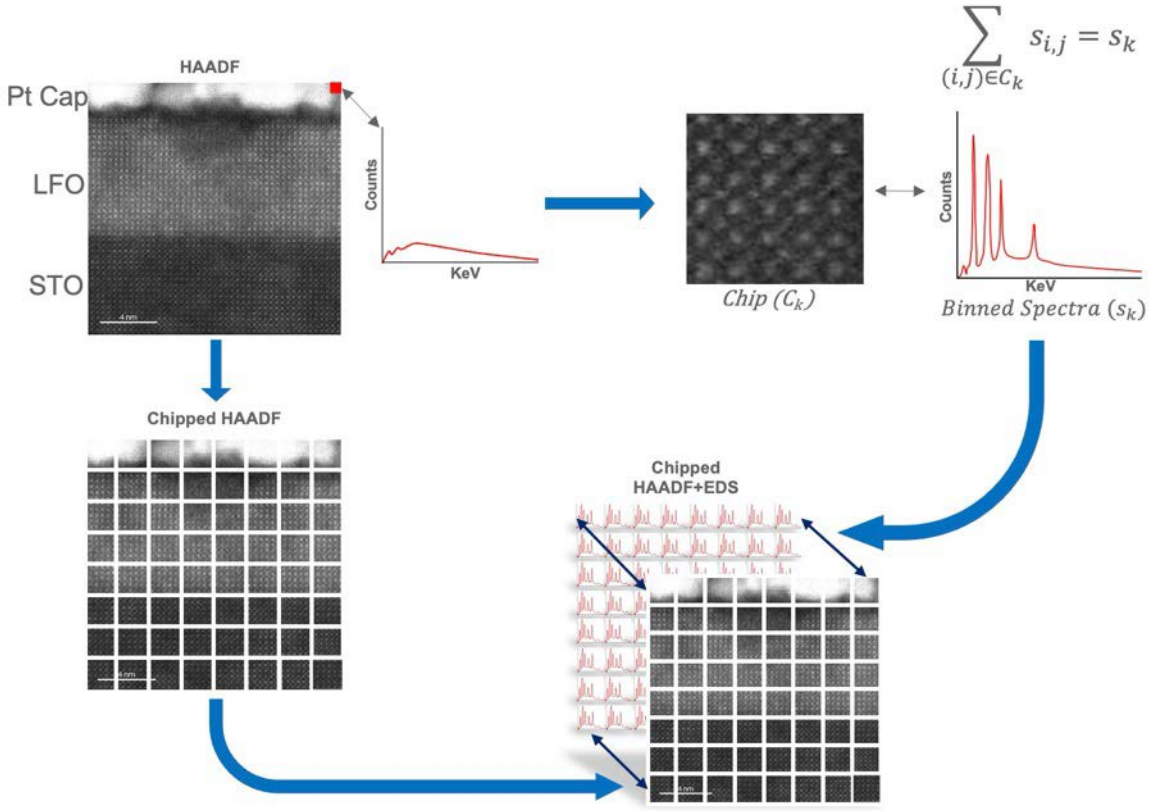
Ter-Petrosyan, A. et al. arXiv (2024). 10.48550/arXiv.2411.09896

Each image pixel is registered to an EDS spectrum that together encode structure and composition.



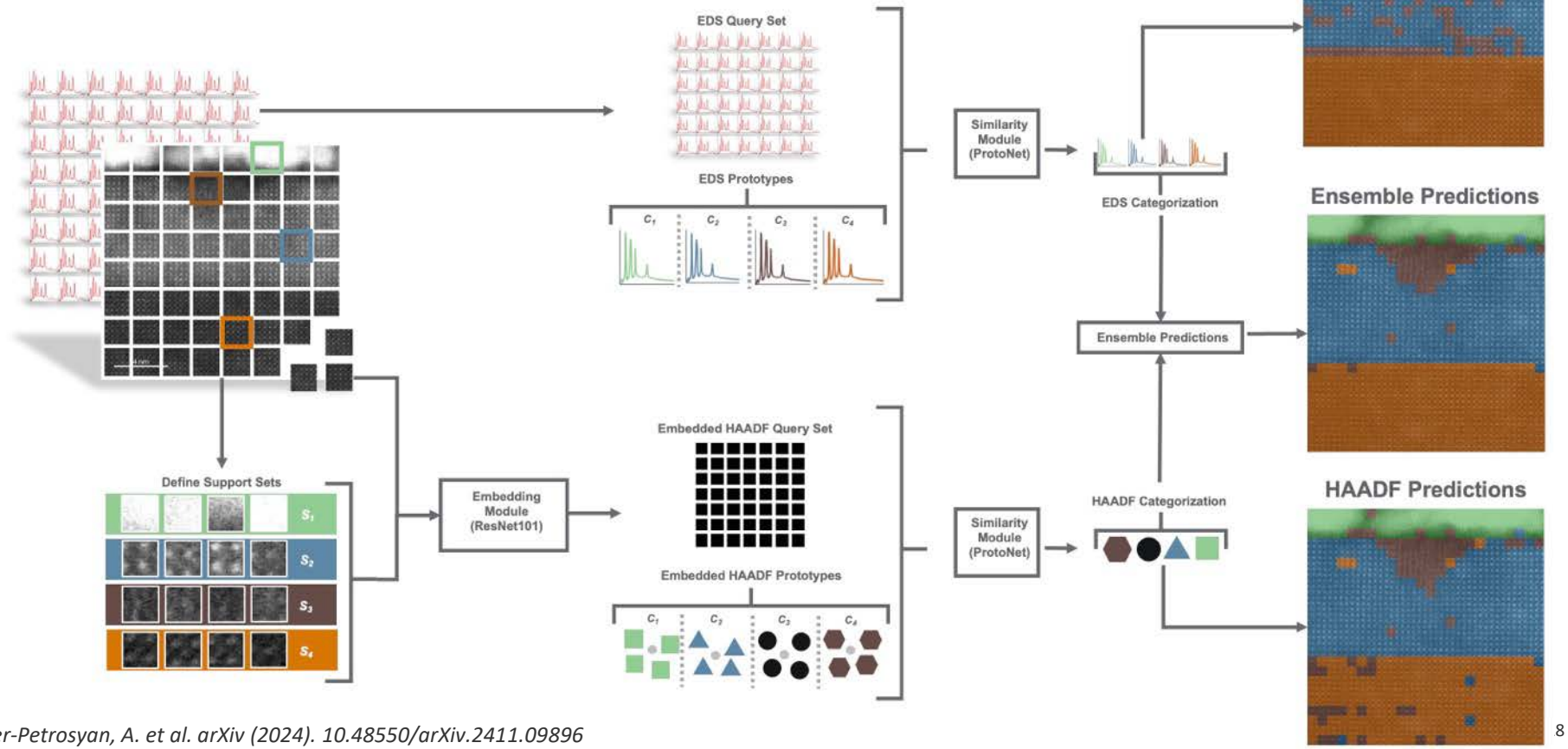
Ter-Petrosyan, A. et al. arXiv (2024). 10.48550/arXiv.2411.09896

To deal with the sparsity of EDS data, we bin the spectra within a regular array.



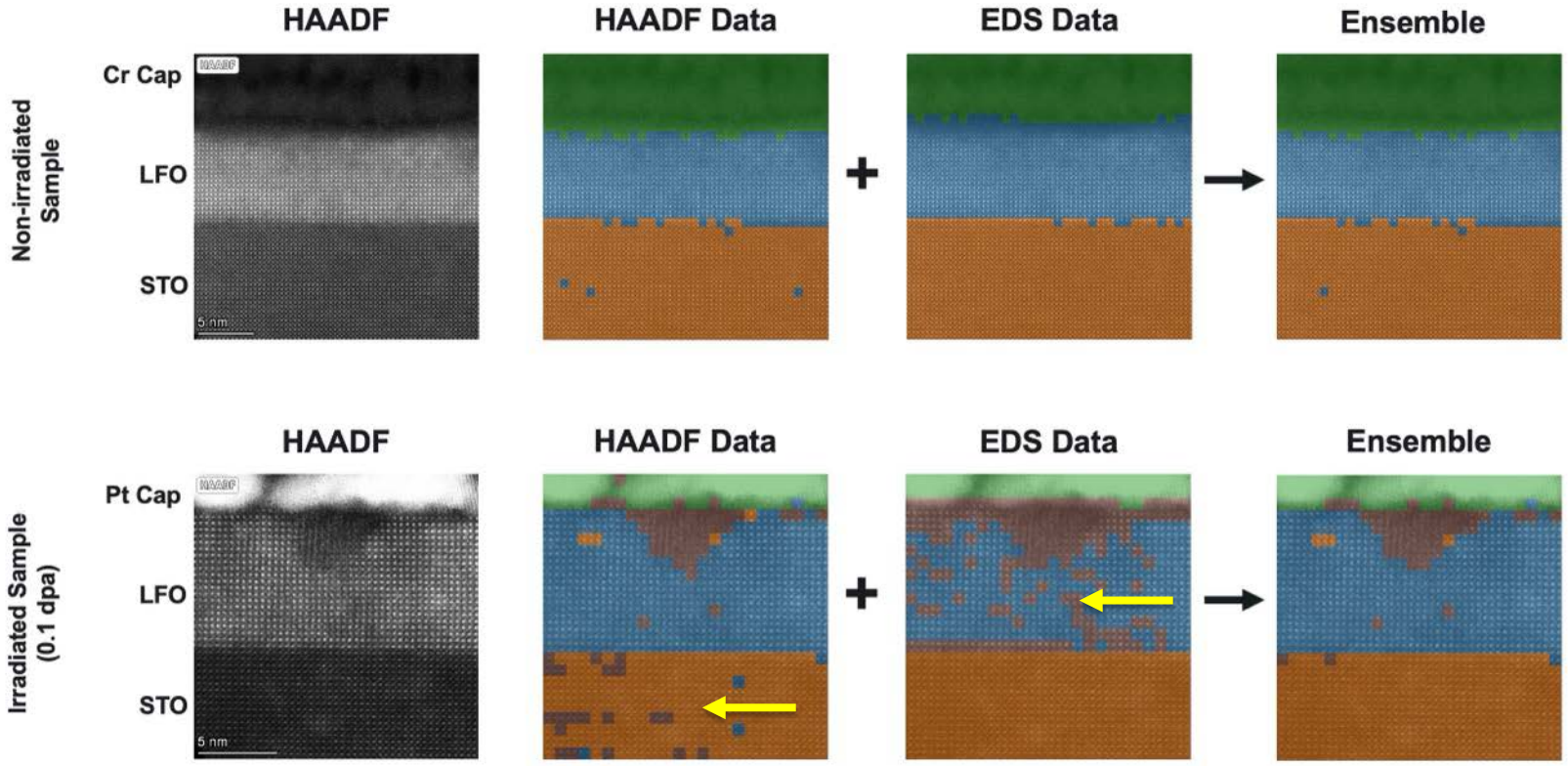
Ter-Petrosyan, A. et al. arXiv (2024). 10.48550/arXiv.2411.09896

We will first focus on a few-shot based approach to classification.



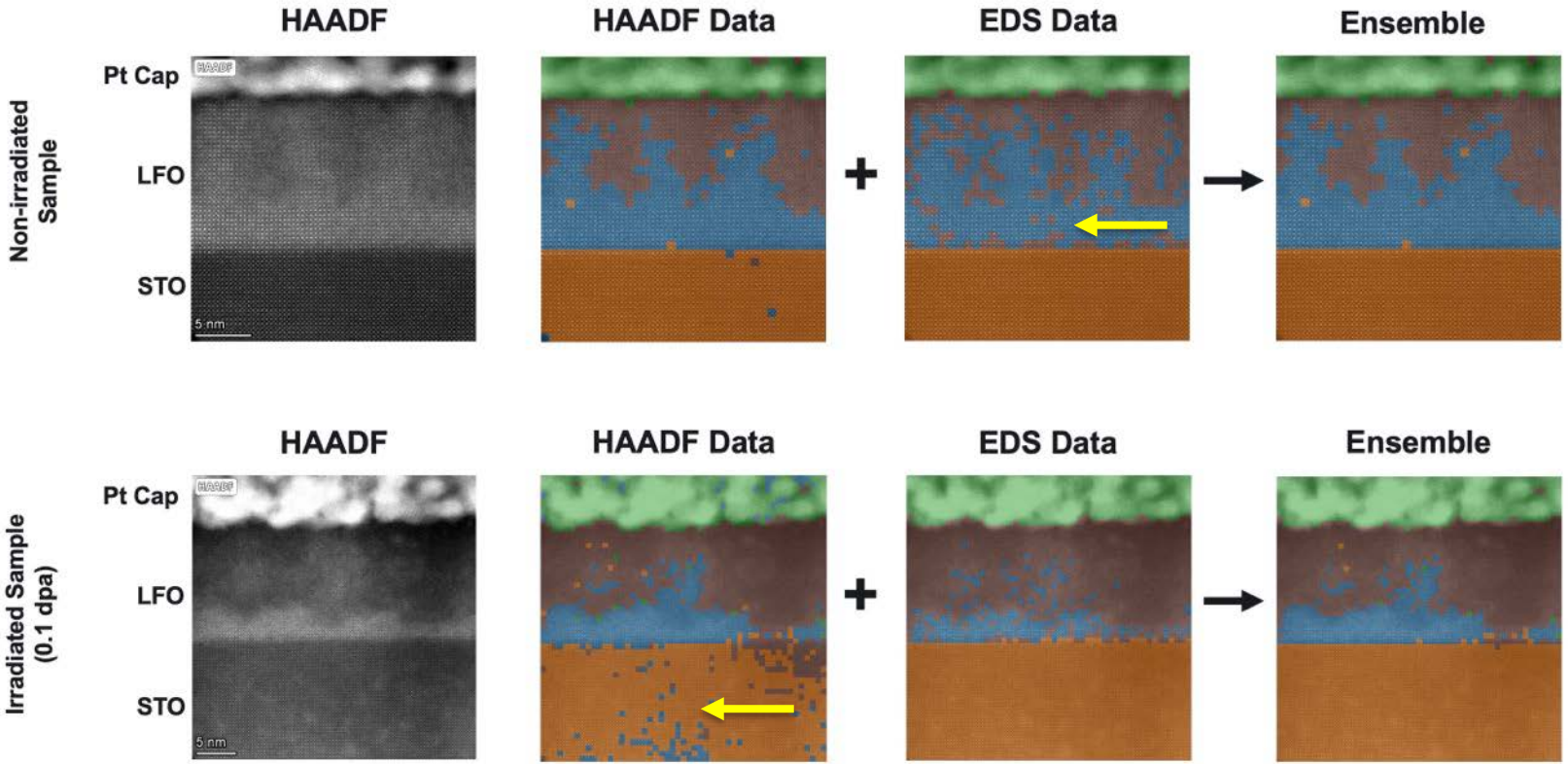
Ter-Petrosyan, A. et al. arXiv (2024). 10.48550/arXiv.2411.09896

For the “pristine” sample, the ensemble model outperforms, especially in more complex microstructures.



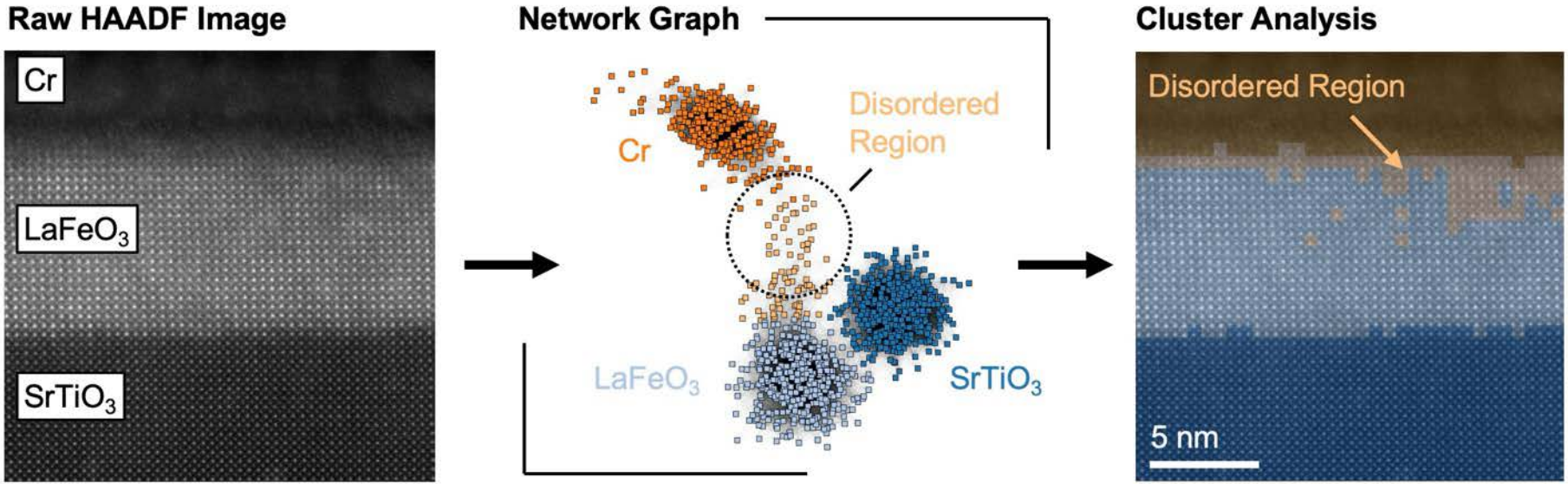
Ter-Petrosyan, A. et al. arXiv (2024). 10.48550/arXiv.2411.09896

The “defective” sample, which consists of more complex domains, shows this even more clearly.

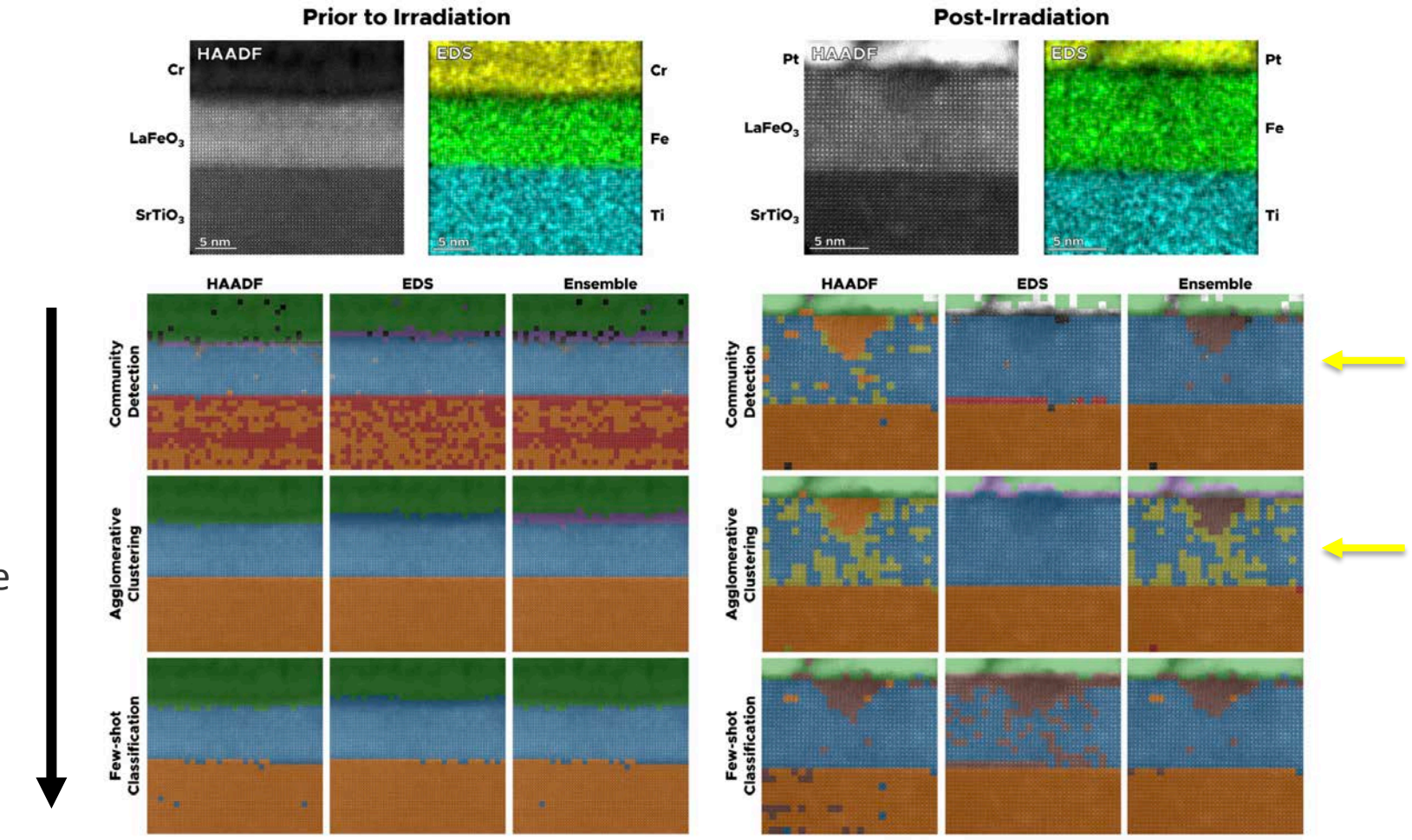


Ter-Petrosyan, A. et al. arXiv (2024). 10.48550/arXiv.2411.09896

But what if we have no a priori knowledge of our sample?

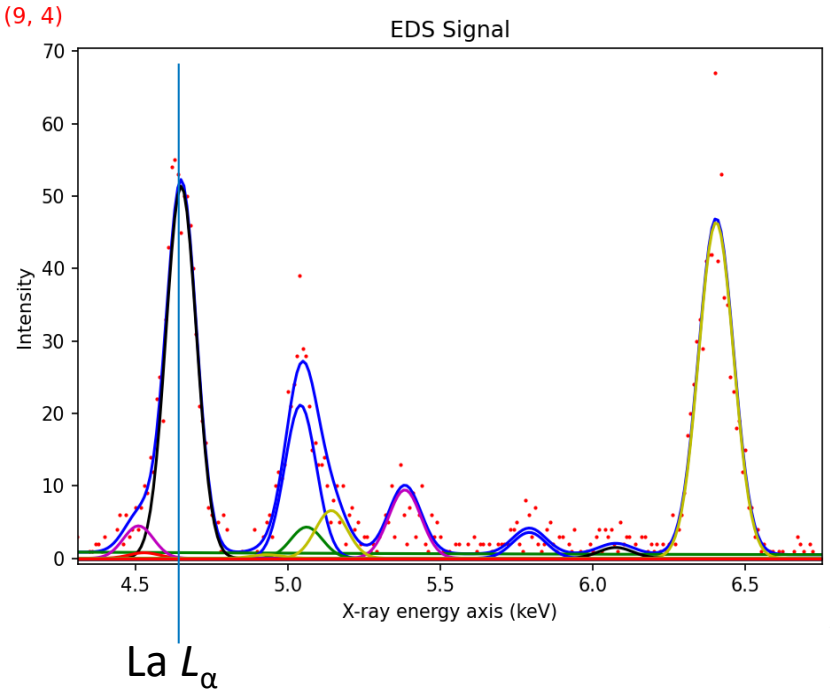


Ter-Petrosyan et al. Proc. Thirty-Seventh Conf. on Neural Information Processing Systems (NeurIPS). (2023). DOI:10.48550/arXiv.2311.08585

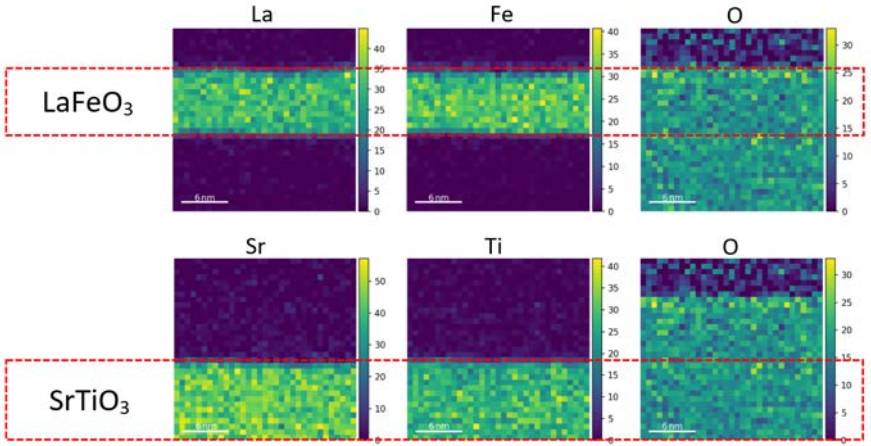


Ter-Petrosyan, A. et al. arXiv (2024). 10.48550/arXiv.2411.09896

The resulting EDS segmentation mask can be quantified using a custom analysis routine.



Benchmarked to known substrate stoichiometry

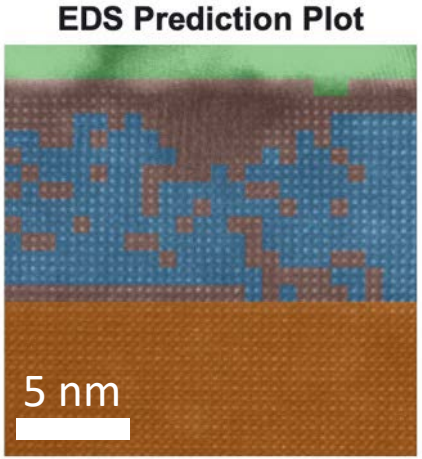


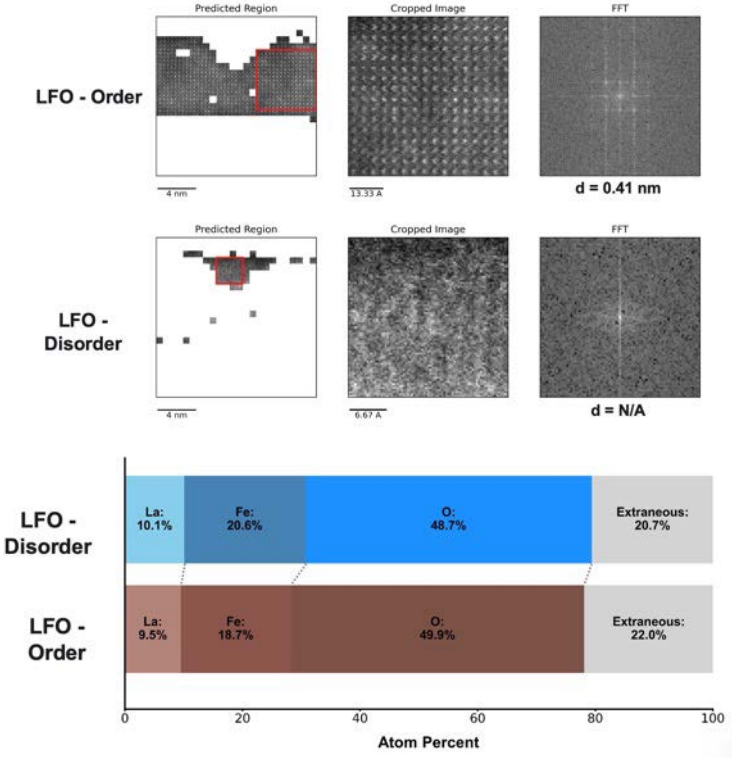
HyperSpy

Open source Python framework for exploring, visualizing and analyzing multi-dimensional data

Get Started

From the predicted masks, we can determine local lattice parameters and composition changes.

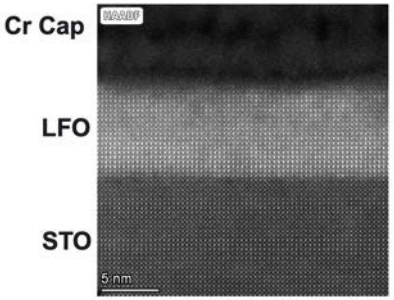




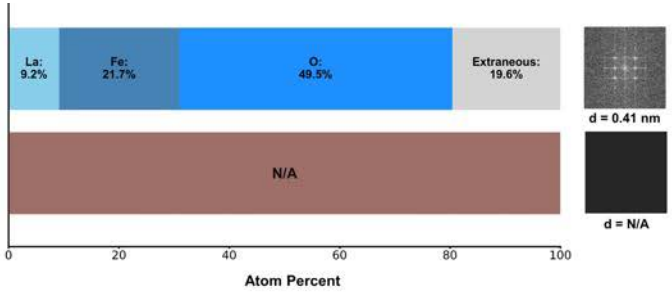
Ter-Petrosyan, A. et al. arXiv (2024). 10.48550/arXiv.2411.09896

We observe distinct trends in alloying element behavior in the disordered regions.

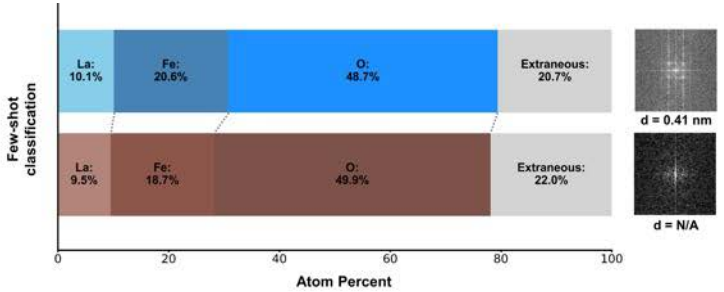
Pristine



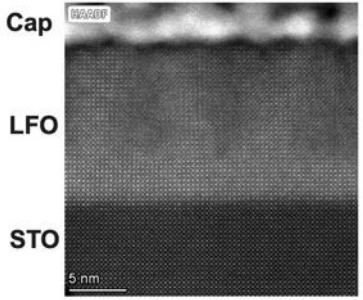
Before Irradiation

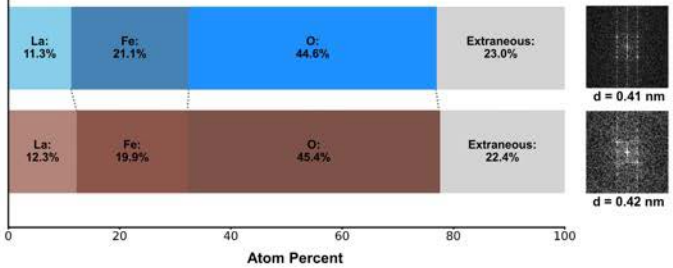


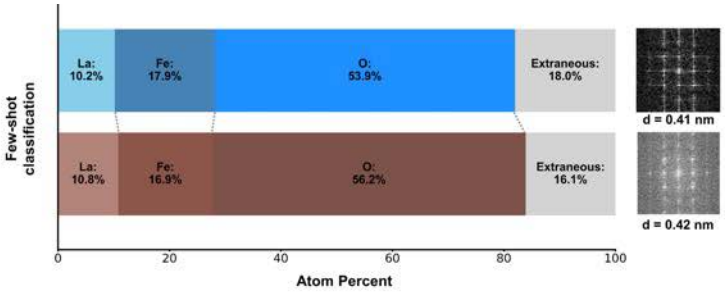
0.1 dpa Irradiation



Defective





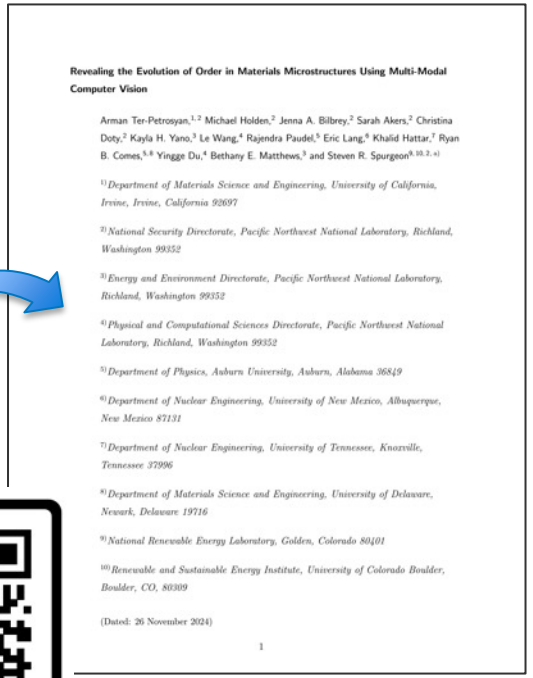


The preserved crystal regions show greater initial Fe and lower O content, pointing toward chemical drivers for disorder.

Ter-Petrosyan, A. et al. arXiv (2024). 10.48550/arXiv.2411.09896

Some key takeaways and topics for future study.

- Multimodal AI can generate powerful descriptors of thin films undergoing structural and chemical evolution.
- A lack of suitable encoders for various data modalities limits the adaptation of models from other domains.
- Understanding the sparsity and character of individual datasets is crucial for appropriate weighting within the model.
- Extracting mechanistic insights will require physics-based approaches to quantification and represents a critical area for future work.



Revealing the Evolution of Order in Materials Microstructures Using Multi-Modal Computer Vision

Arman Ter-Petrosyan,[1,2] Michael Holden,[2] Jenna A. Bilbrey,[2] Sarah Akers,[2] Christina Doty,[2] Kayla H. Yano,[3] Le Wang,[4] Rajendra Paudel,[5] Eric Lang,[6] Khalid Hattar,[7] Ryan B. Comes,[5,8] Yingge Du,[4] Bethany E. Matthews,[3] and Steven R. Spurgeon[9,10,2,*]

[1] *Department of Materials Science and Engineering, University of California, Irvine, Irvine, California 92697*

[2] *National Security Directorate, Pacific Northwest National Laboratory, Richland, Washington 99352*

[3] *Energy and Environment Directorate, Pacific Northwest National Laboratory, Richland, Washington 99352*

[4] *Physical and Computational Sciences Directorate, Pacific Northwest National Laboratory, Richland, Washington 99352*

[5] *Department of Physics, Auburn University, Auburn, Alabama 36849*

[6] *Department of Nuclear Engineering, University of New Mexico, Albuquerque, New Mexico 87131*

[7] *Department of Nuclear Engineering, University of Tennessee, Knoxville, Tennessee 37996*

[8] *Department of Materials Science and Engineering, University of Delaware, Newark, Delaware 19716*

[9] *National Renewable Energy Laboratory, Golden, Colorado 80401*

[10] *Renewable and Sustainable Energy Institute, University of Colorado Boulder, Boulder, CO, 80309*

(Dated: 26 November 2024)

1

SCAN ME

Download the preprint at:
doi.org/10.48550/arXiv.2411.09896

The Team

PNNL

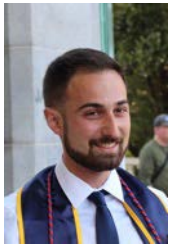
Jenna Pope

Christina Doty

Sarah Akers

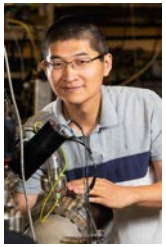
Yingge Du

Bethany Matthews



Arman Ter-Petrosyan
Now: Ph.D. at UCI

Mike Holden



Le Wang

UTK

Khalid Hattar

UDel

Ryan Comes

UNM

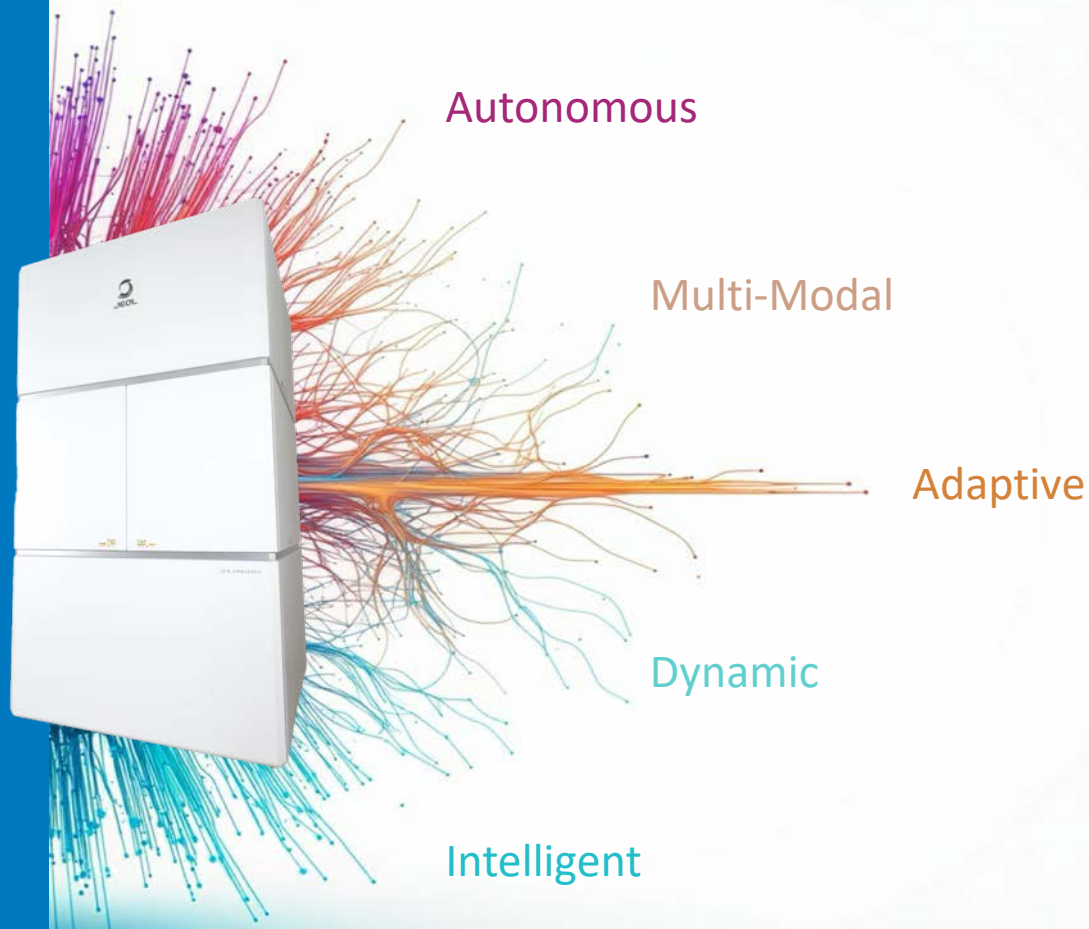
Eric Lang

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

Work with us!

DOE Science Undergraduate Laboratory Internships (SULI)

- Internship Dates: Fall 2025
- Application Due: TBD / Closer to Summer
- Apply: https://science.osti.gov/wdts/suli

DOE Office of Science Graduate Student Research (SCGSR) Program

- Program Duration: Up to 12 months
- Application Due: May 7, 2025
- Apply: https://science.osti.gov/wdts/scgsr

Co-Op Intern Addie Salvador (Top)
Postdoc Michelle Smeaton (Middle)
SULI Student Grace Guinan (Bottom)

See our related computer vision work in the poster session tonight!

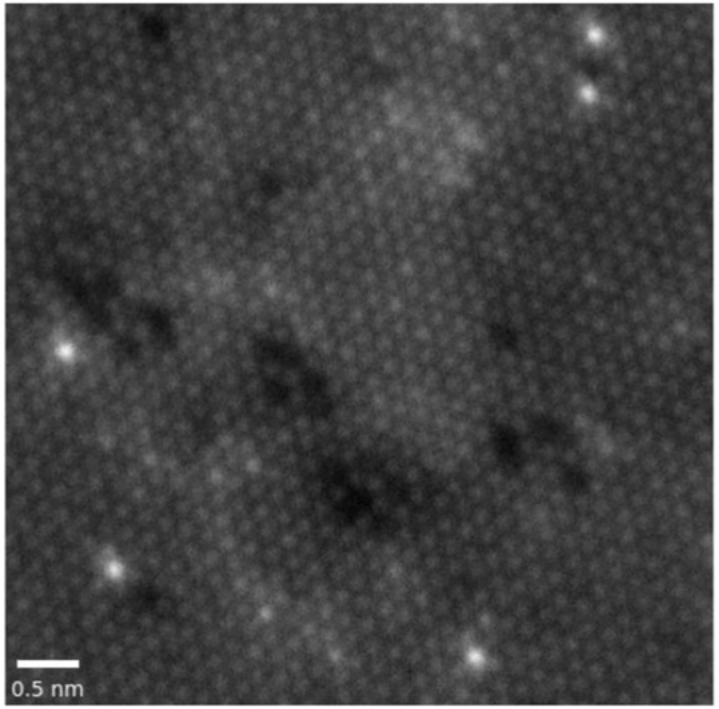
Accelerating Discovery of Atomistic Defects via Machine Learning

Applying computer vision to classification of point defects in 2D materials.

Author: Grace Guinan

Location: Penrose Ballroom

Time: 5:30-7:00 pm



NREL

COLORADO SCHOOL OF MINES

AI models have the potential to reveal hidden materials lifecycles from multimodal data, transforming the design of thin films.

Contact Me:
steven.spurgeon@nrel.gov

SCAN ME

NREL/PR-5K00-93479

This work was authored by NREL for the U.S. Department of Energy (DOE), operated under Contract No. DE-AC36-08GO28308. S.R.S. was supported by the O2O: Operando to Operation transformative laboratory directed research and development (LDRD) program at NREL. The views expressed in the presentation do not necessarily represent the views of the DOE or the U.S. Government. The U.S. Government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this work, or allow others to do so, for U.S. Government purposes. The development of the multimodal model was supported by the LDRD program at Pacific Northwest National Laboratory (PNNL). PNNL is a multiprogram national laboratory operated for the U.S. DOE by Battelle Memorial Institute under Contract No. DE-AC05-76RL0-1830. In situ ion irradiation work was performed at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. DOE. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE's National Nuclear Security Administration under contract DE-NA- 0003525.