Beyond the Hype
Navigating the Promise and Pitfalls of Multi-Modal Models for Materials Science

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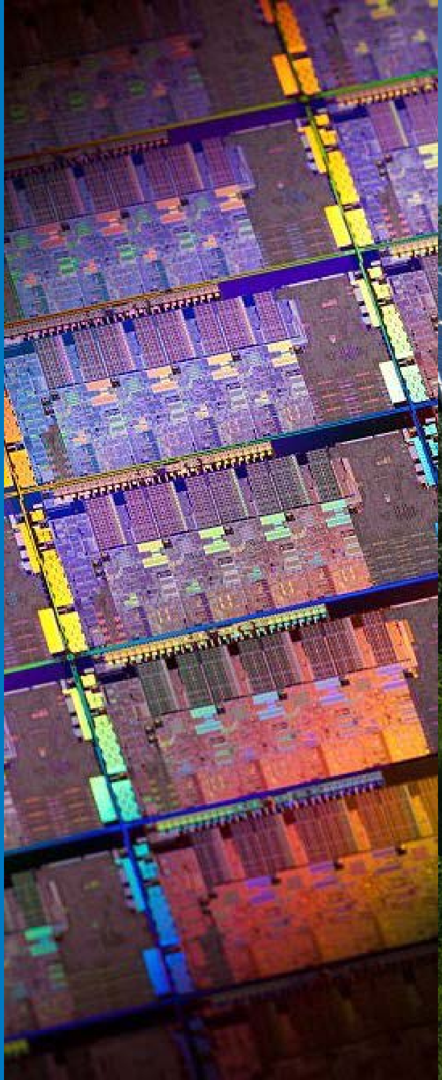
MRS Fall 2024

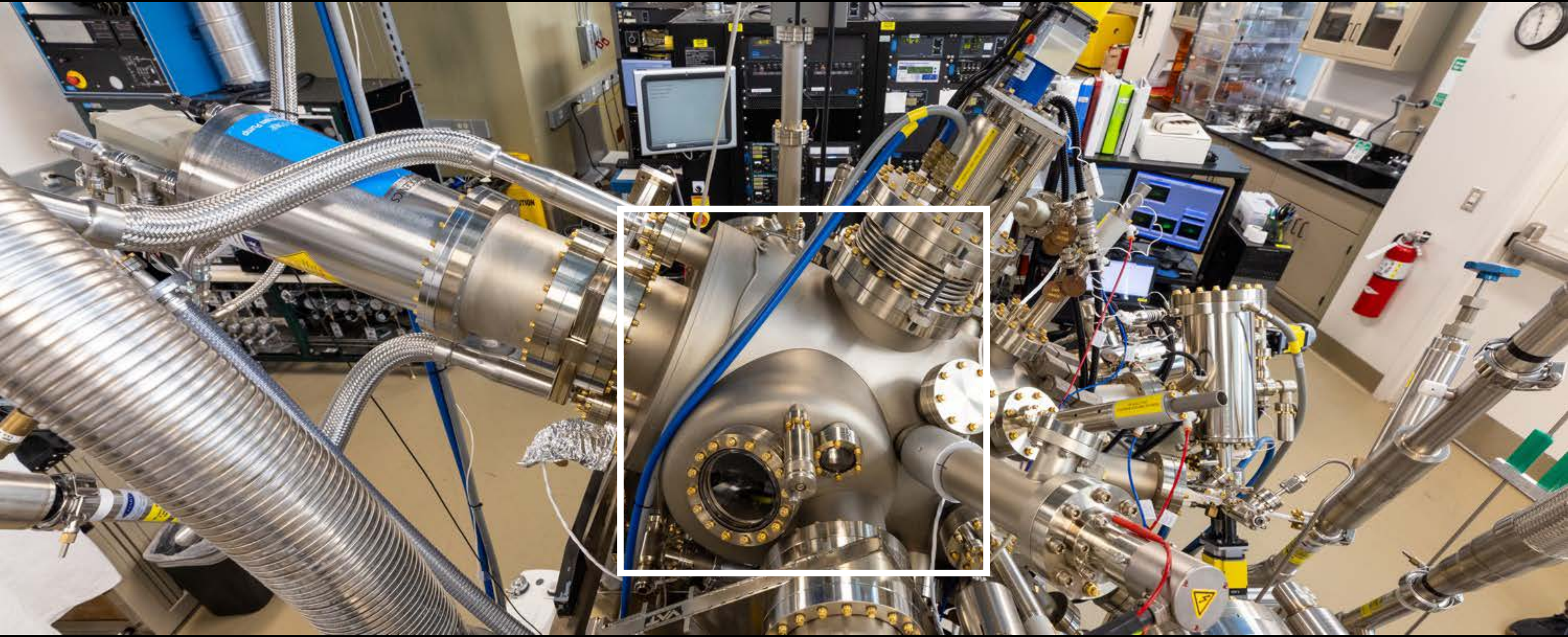
December 2, 2024

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.

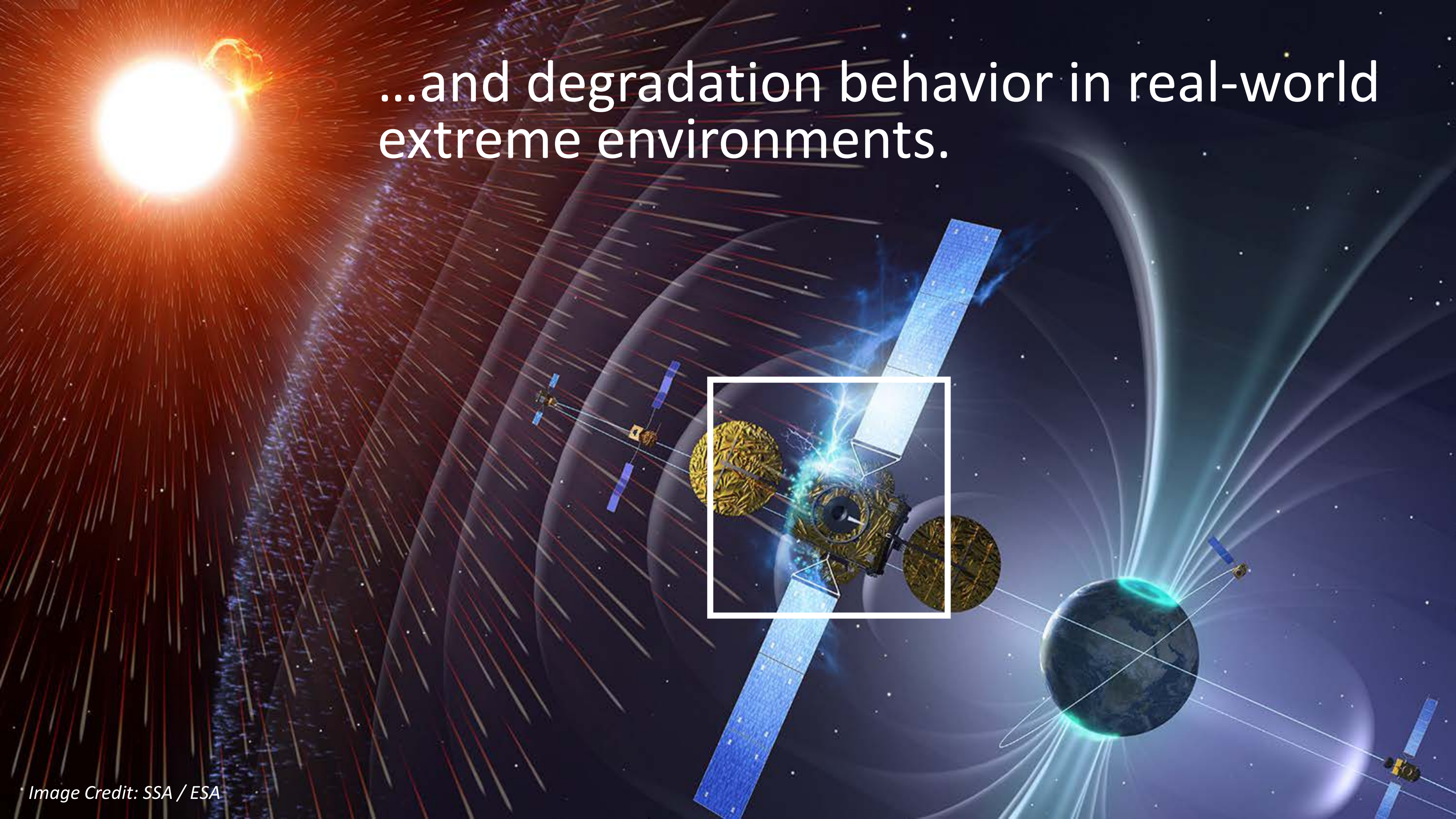
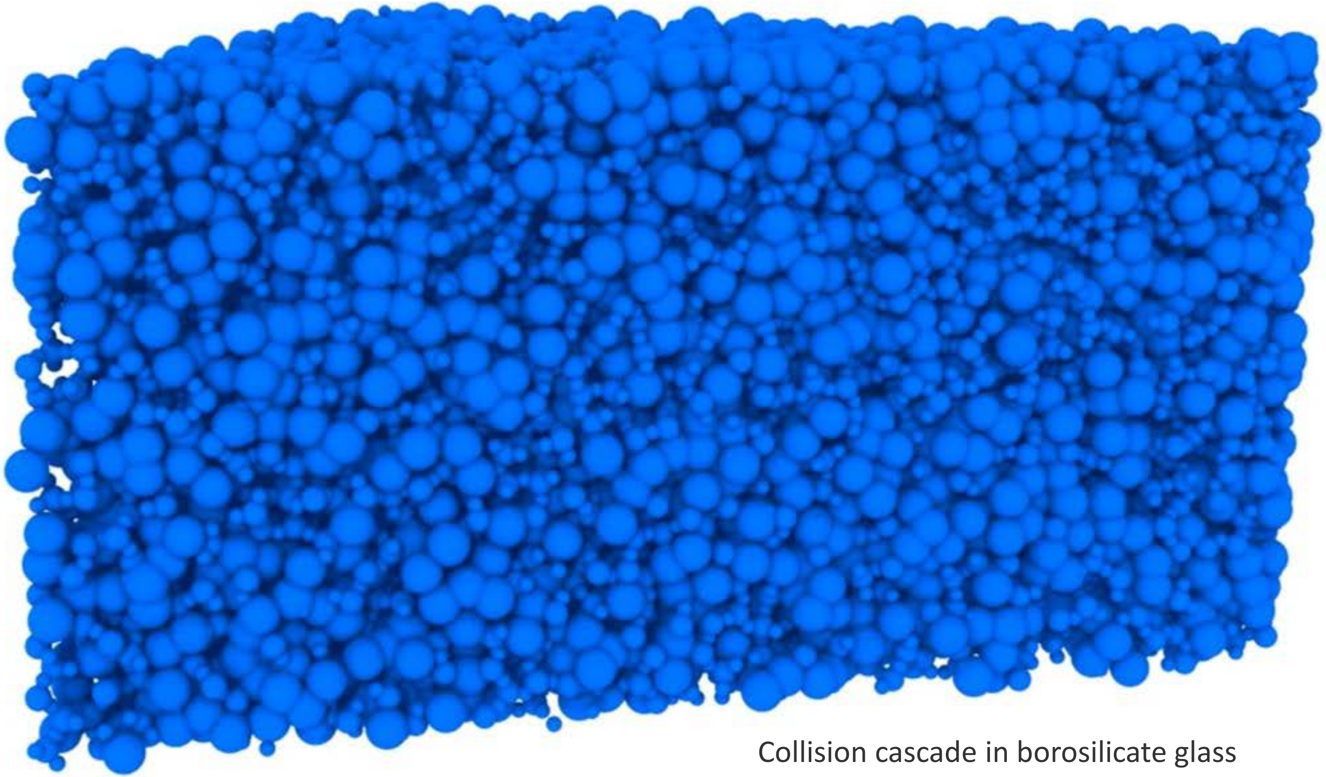


Image Credit: SSA / ESA

…and degradation behavior in real-world extreme environments.



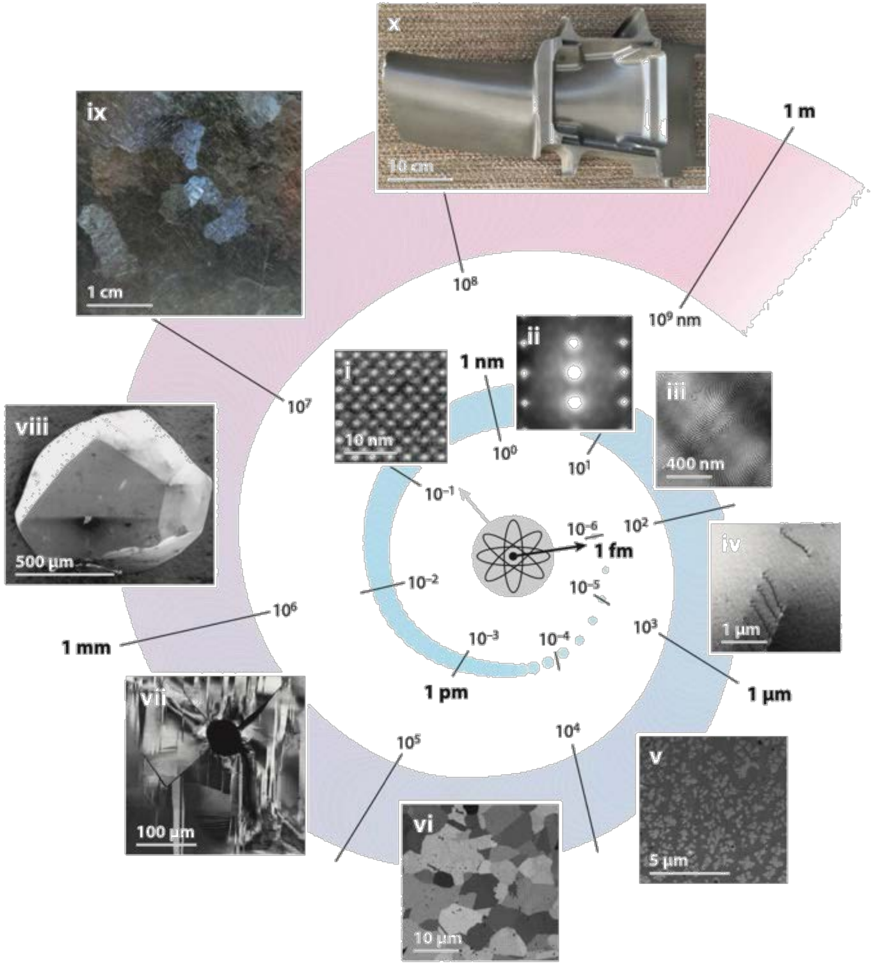
Collision cascade in borosilicate glass

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

My research aim is an ontology of the materials lifecycle:

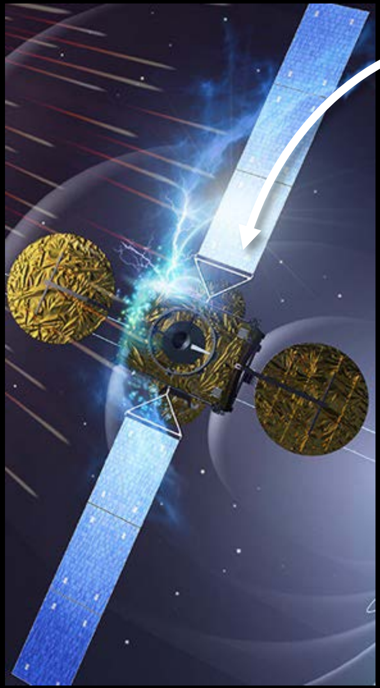
*"A systematic mapping of data to meaningful semantic concepts…" **across spatial and temporal scales***

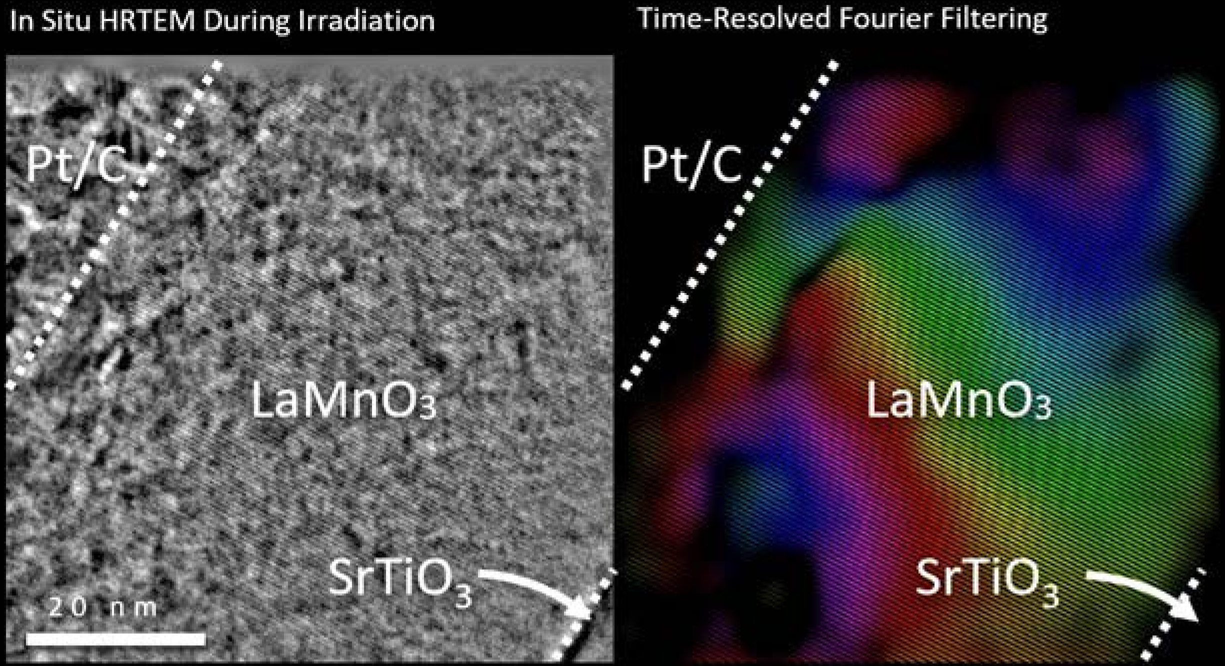
Quote adapted from: https://blog.palantir.com/ontology-finding-meaning-in-data-palantir-rfx-blog-series-1-399bd1a5971b



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.



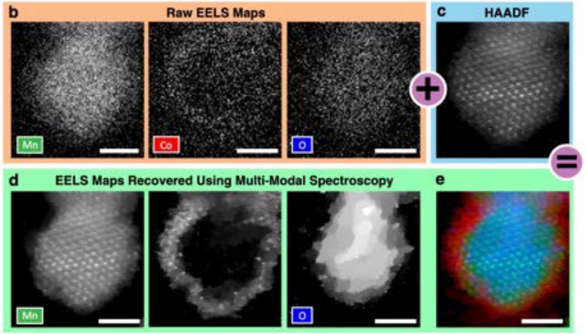


- What are the fundamental principles relating interfaces and radiation-induced defects?
- Can we derive an order parameter that describes the disordering process enabling more robust design of oxide-based devices?

Image Credit: SSA / ESA | Matthews et al. Nano Letters, 21(12), 5353–5359. (2021).

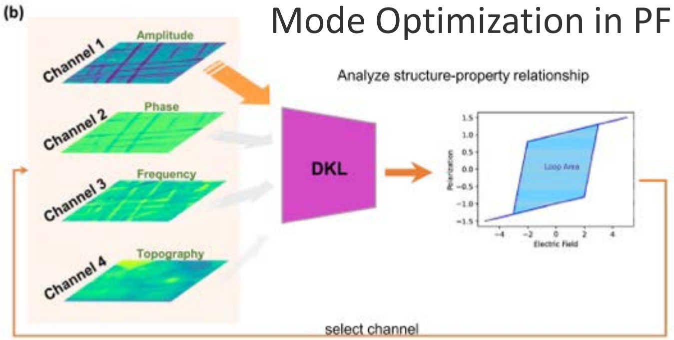
Multi-modal models provide a potentially powerful window into the materials lifecycle.

Fused Multi-Modal STEM



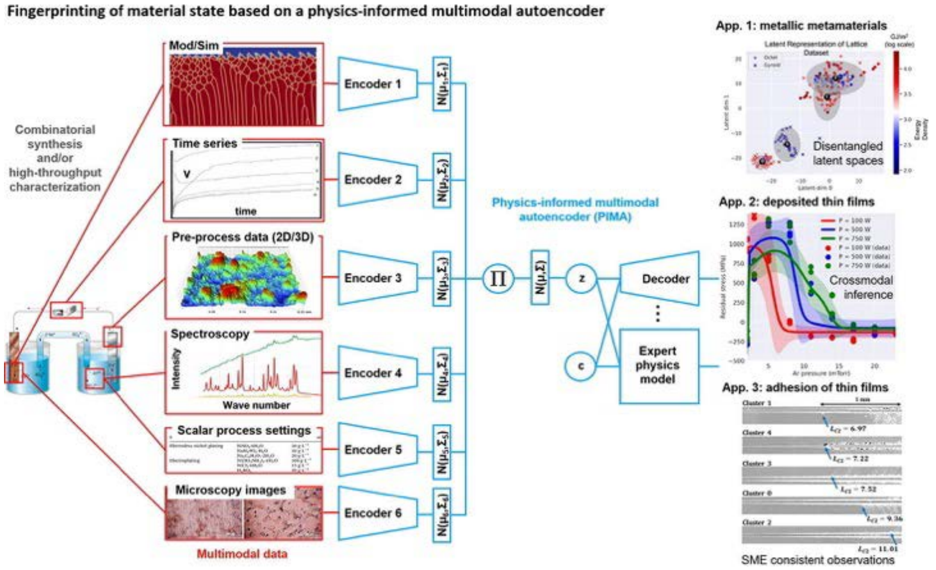
Schwartz et al. npj Comp. Mater. 8, 16 (2022).

Mode Optimization in PFM



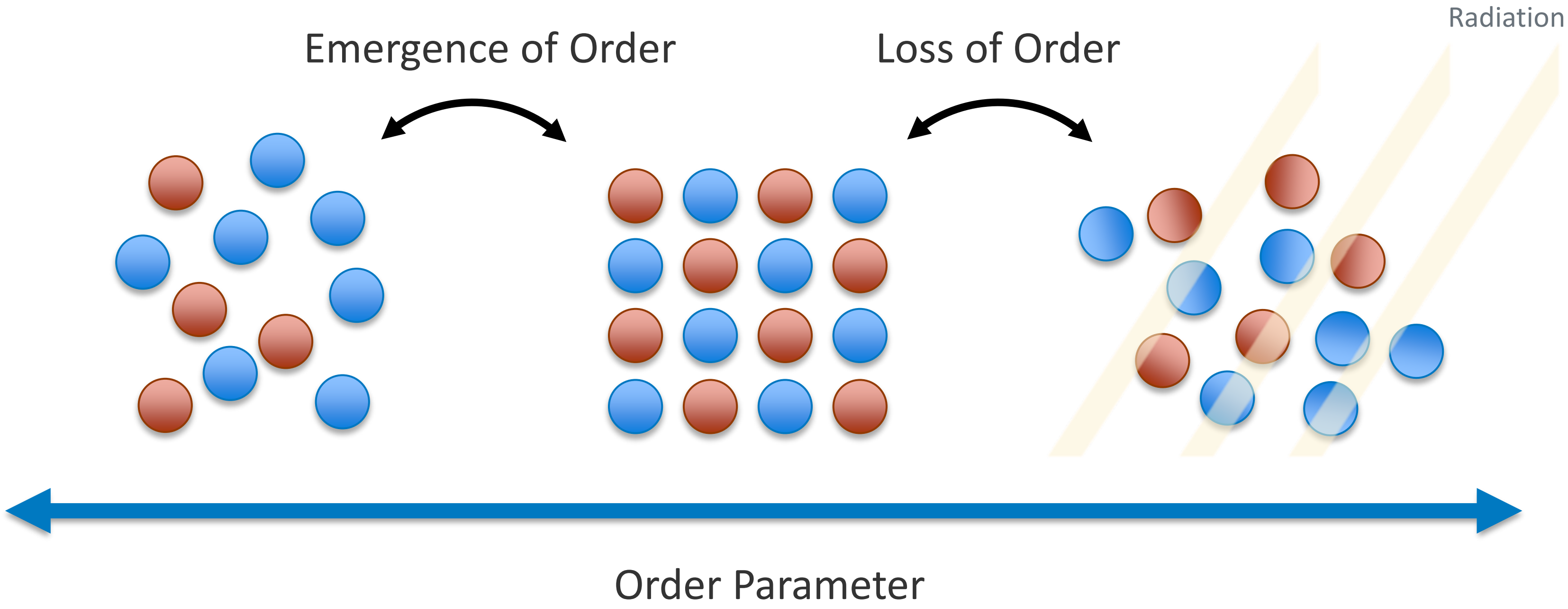
Liu et al. npj Comput. Mater. 9, 34 (2023).

Multi-Modal Autoencoders for Materials

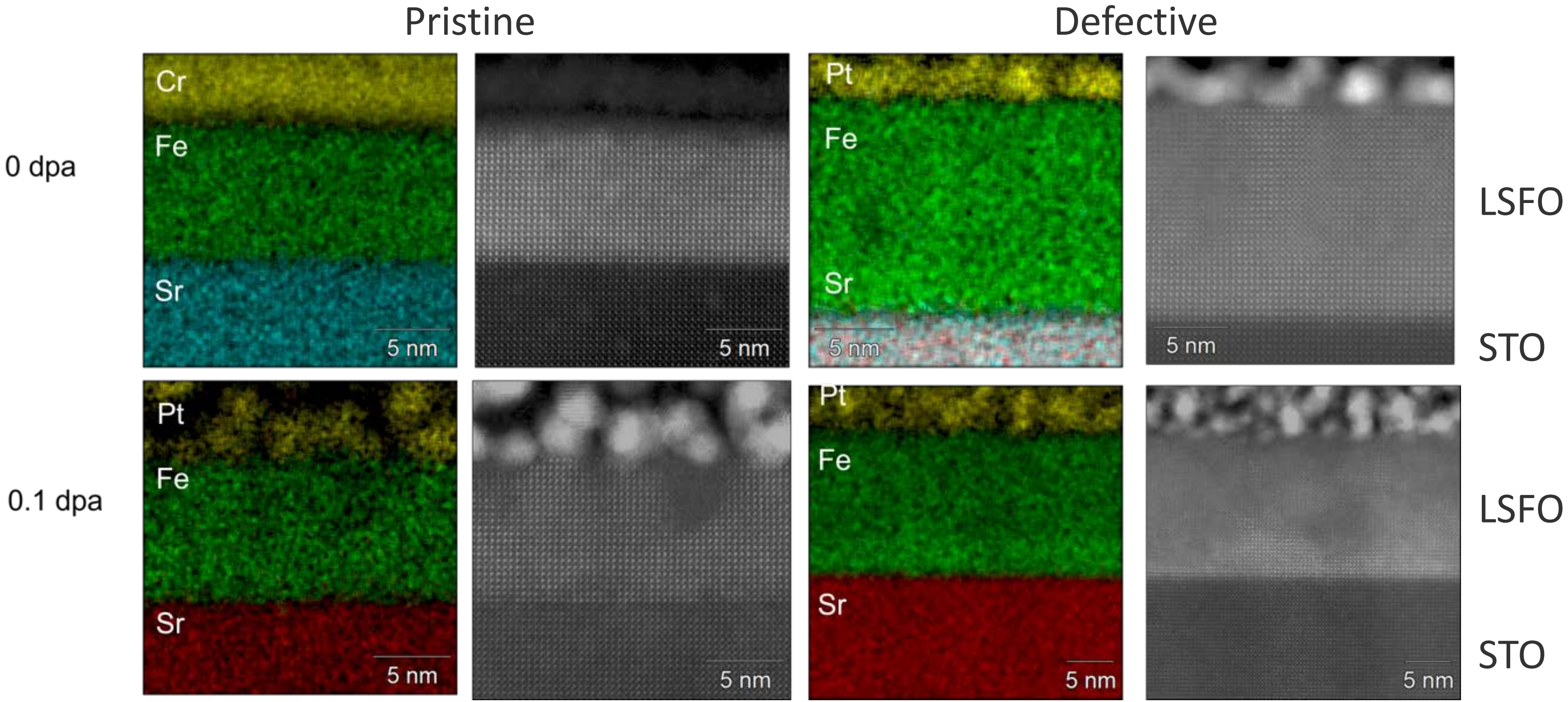


Trask et al. Mater. Today. 80, 286 (2024).

Can these models inform an order parameter for the evolution of crystalline materials?



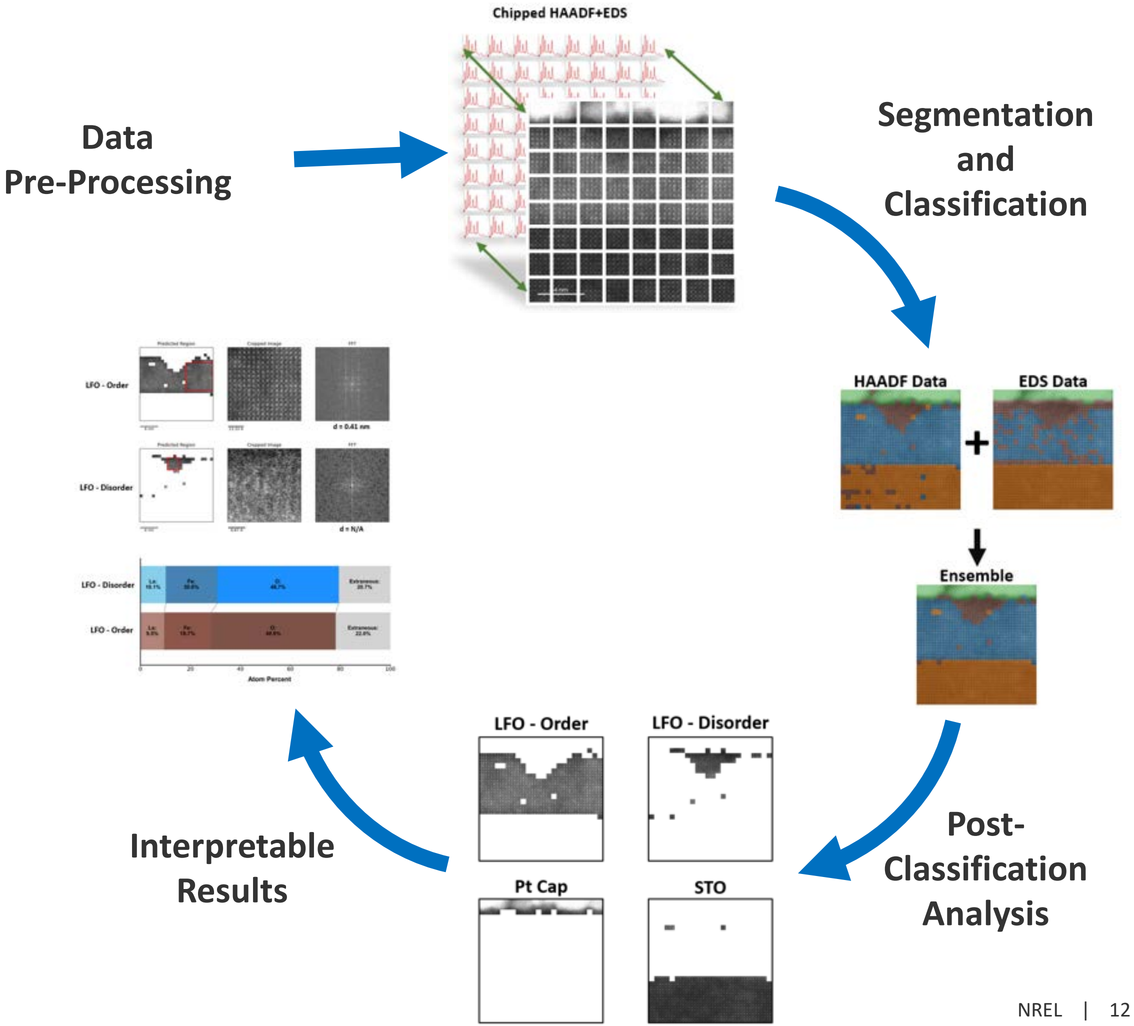
We examine the effect of initial microstructure and vacancy content on disordering pathways in $La_{1-x}Sr_xFeO_3$.



Irradiated with 2.8 MeV Au^{2+} ions

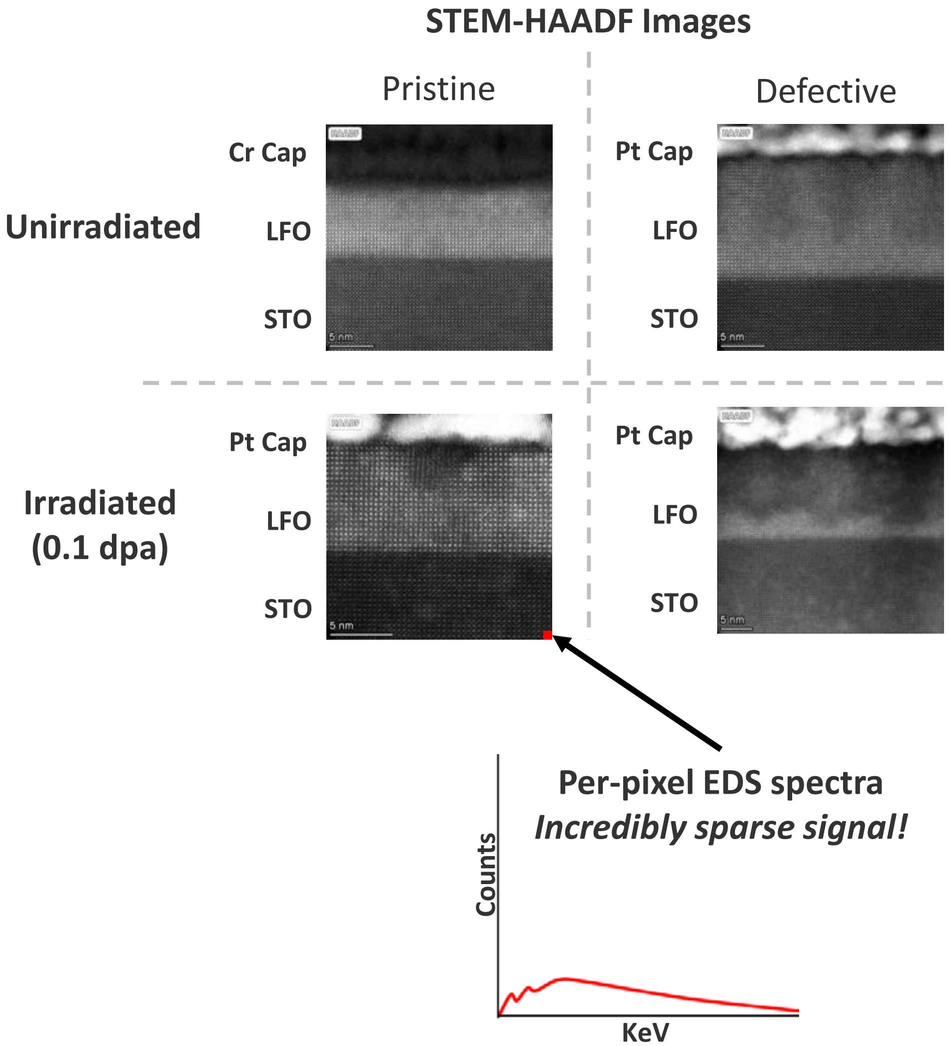
Ter-Petrosyan, A. et al. arXiv (2024). 10.48550/arXiv.2411.09896

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



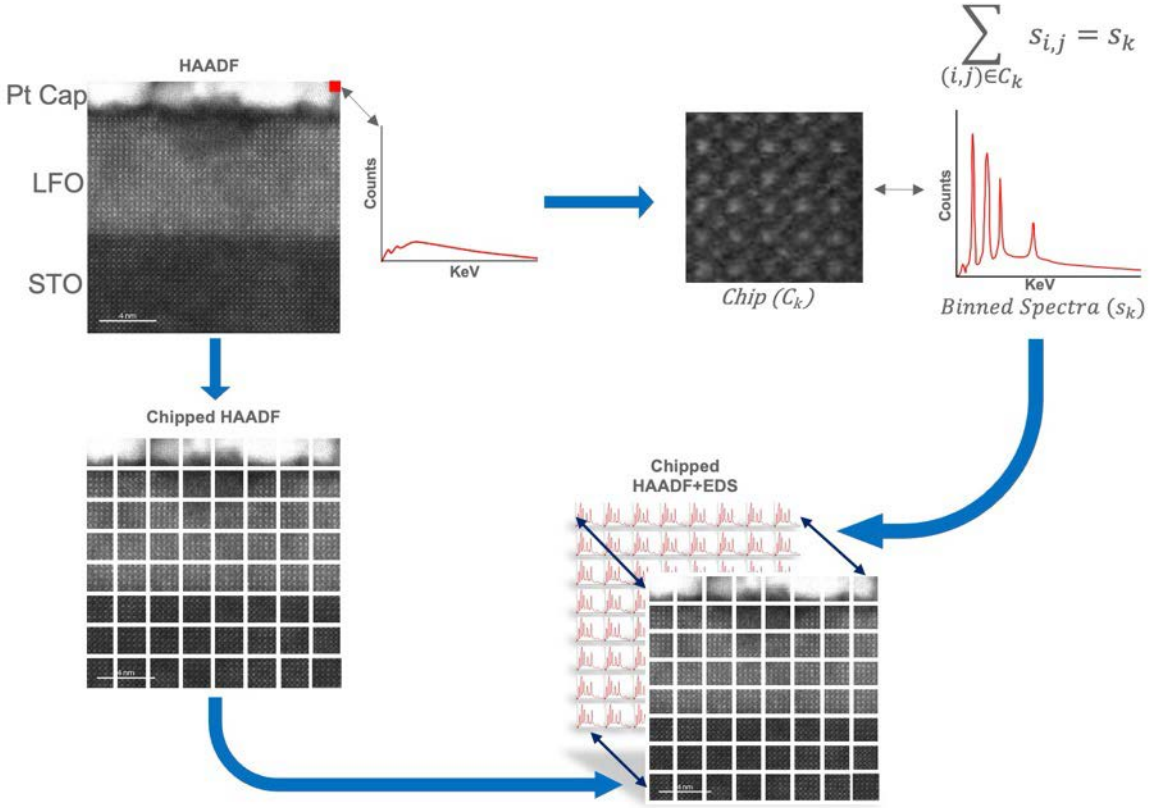
Ter-Petrosyan, A. et al. arXiv (2024). 10.48550/arXiv.2411.09896

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



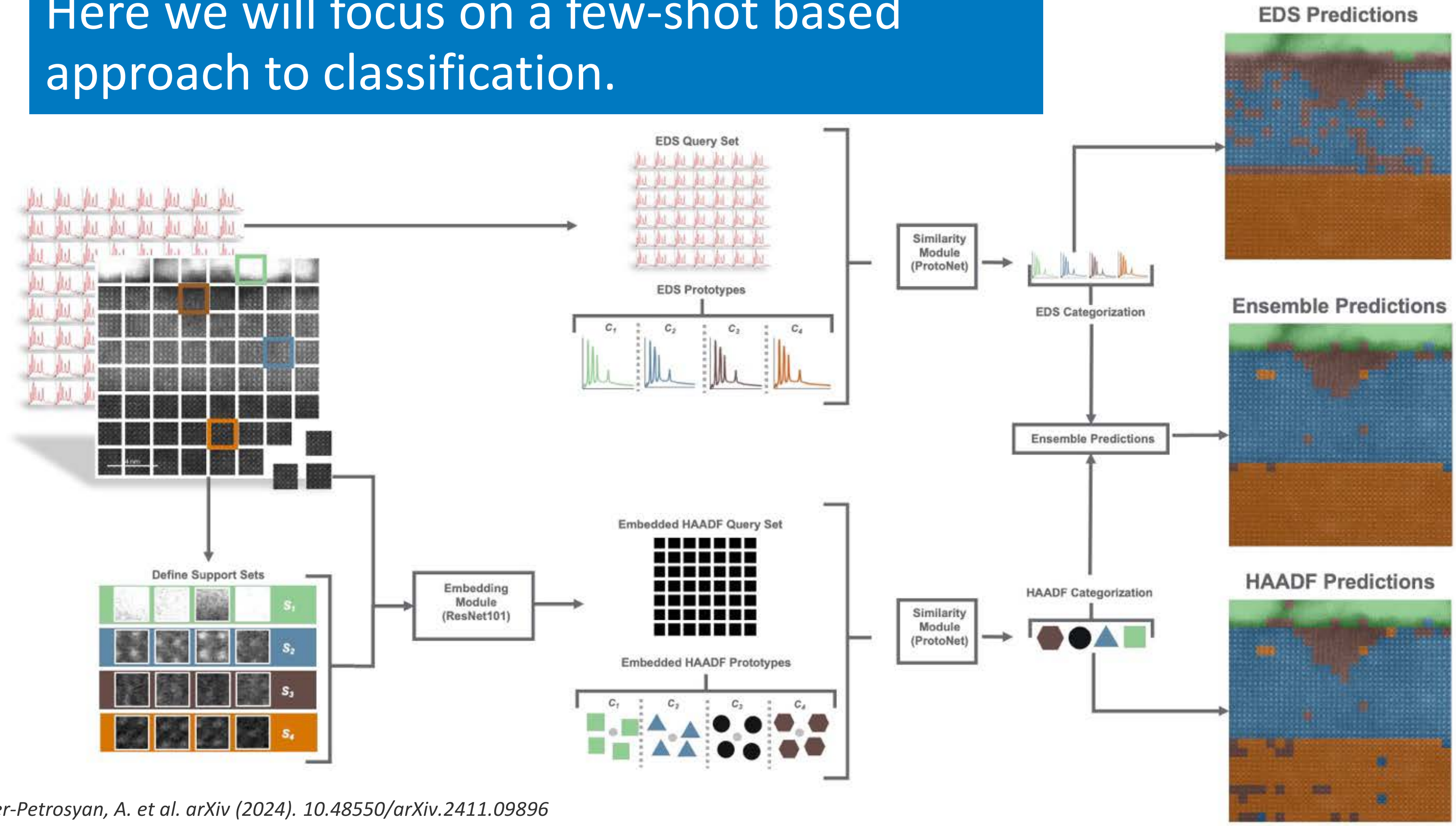
Ter-Petrosyan, A. et al. arXiv (2024). 10.48550/arXiv.2411.09896

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



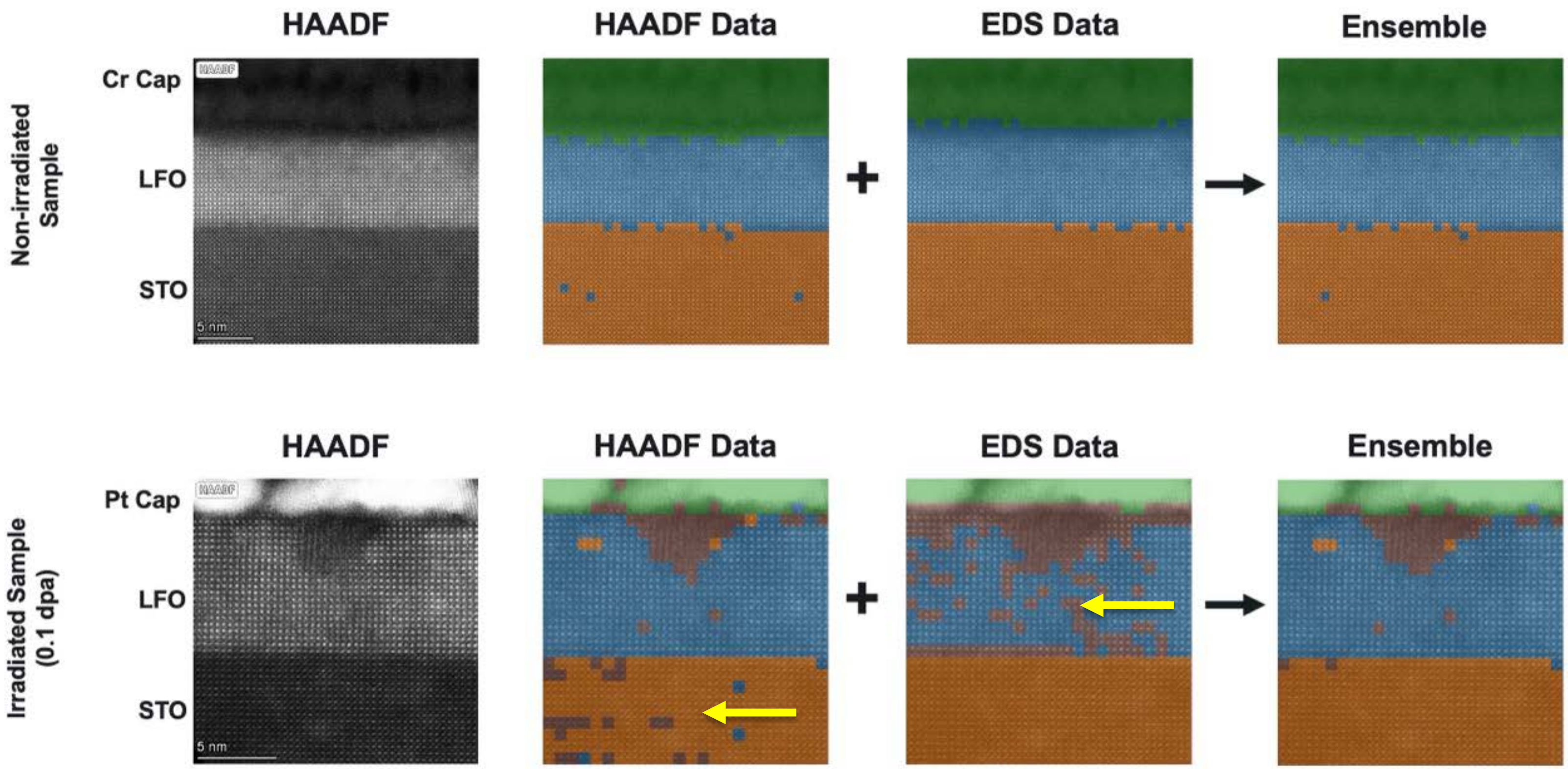
Ter-Petrosyan, A. et al. arXiv (2024). 10.48550/arXiv.2411.09896

Here we will focus on a few-shot based approach to classification.



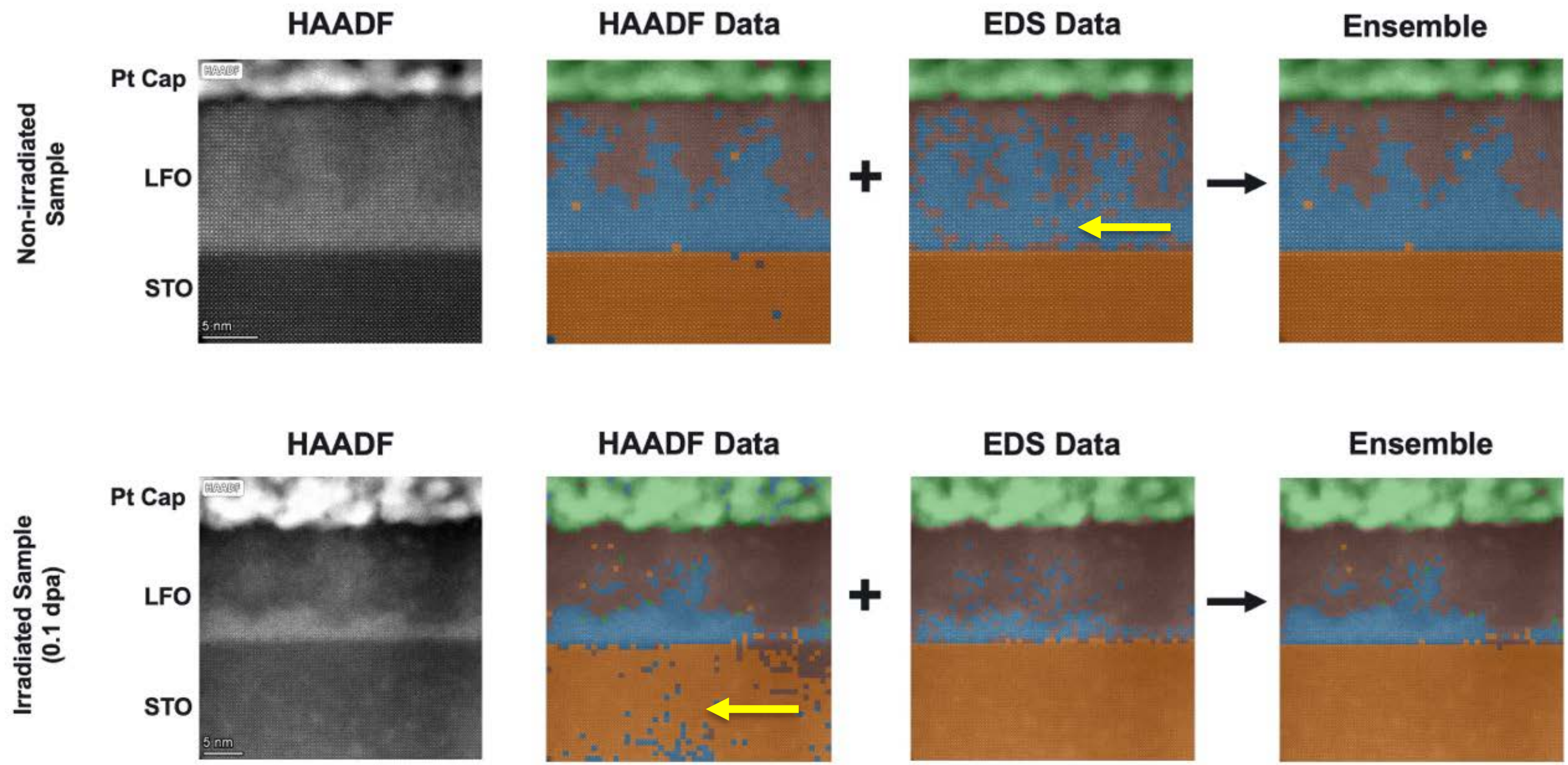
Ter-Petrosyan, A. et al. arXiv (2024). 10.48550/arXiv.2411.09896

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



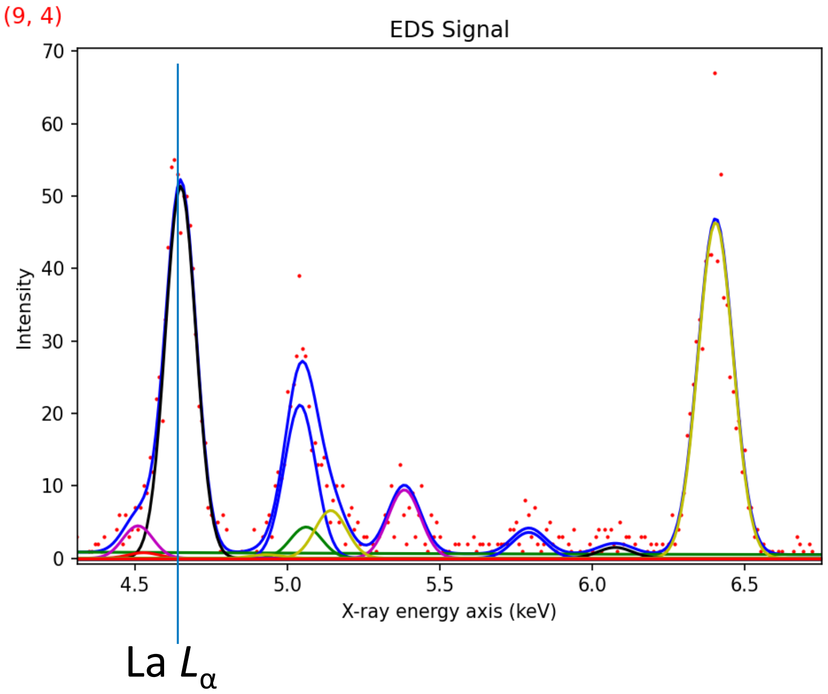
Ter-Petrosyan, A. et al. arXiv (2024). 10.48550/arXiv.2411.09896

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

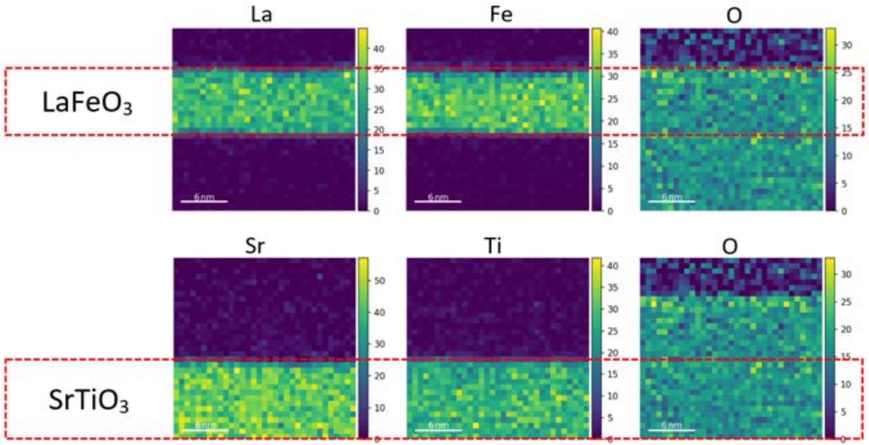


Ter-Petrosyan, A. et al. arXiv (2024). 10.48550/arXiv.2411.09896

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



Benchmarked to known substrate stoichiometry



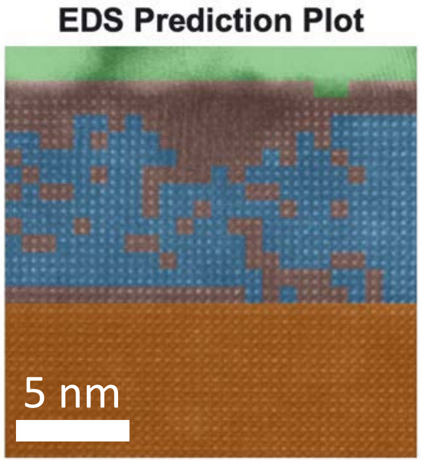
HyperSpy

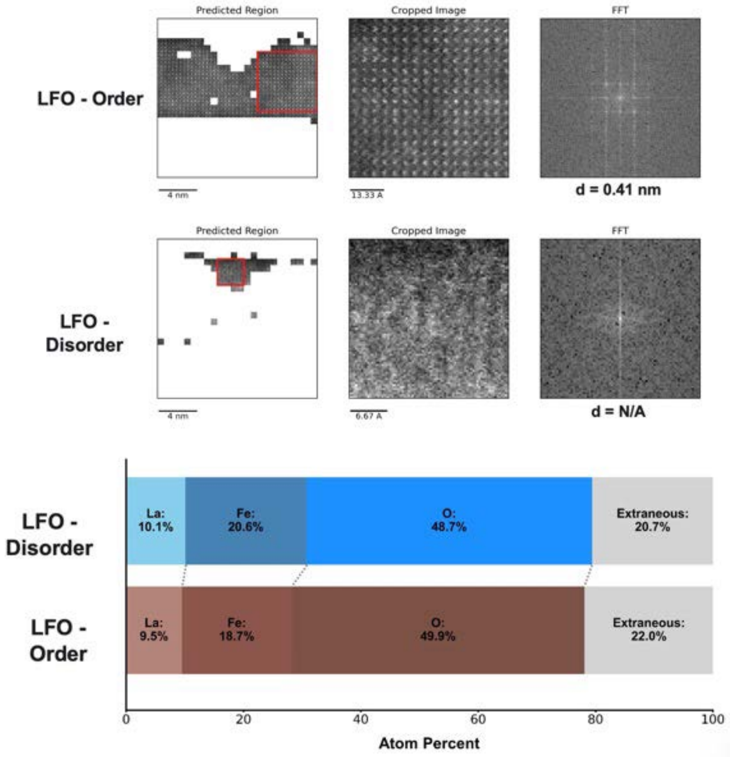
Open source Python framework for exploring, visualizing and analyzing multi-dimensional data

Get Started

Ter-Petrosyan, A. et al. arXiv (2024). 10.48550/arXiv.2411.09896 | https://hyperspy.org/index.html

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

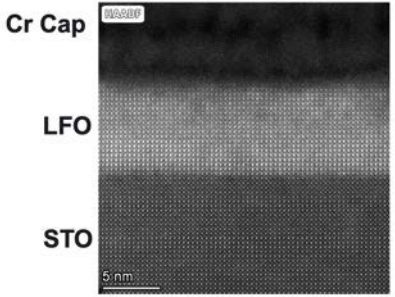




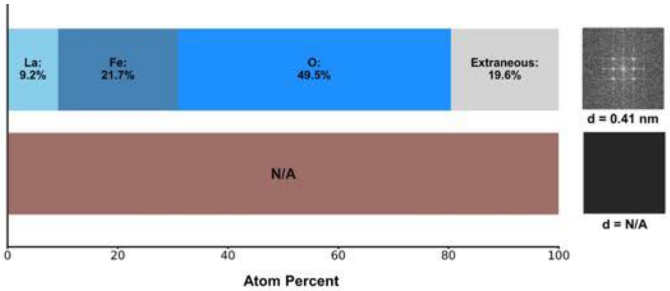
Ter-Petrosyan, A. et al. arXiv (2024). 10.48550/arXiv.2411.09896

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

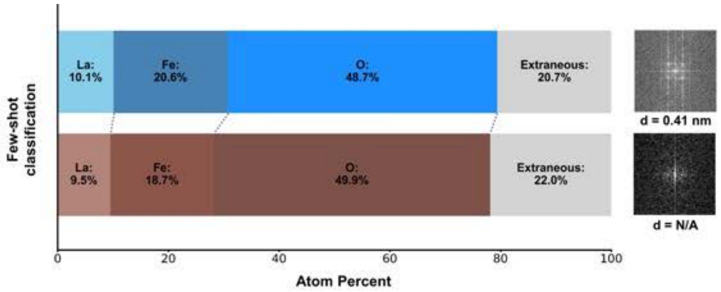
Pristine



Before Irradiation

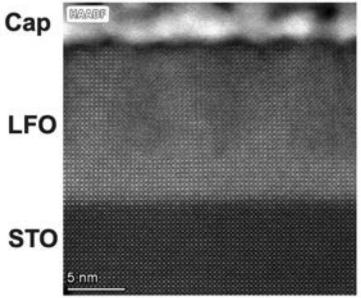


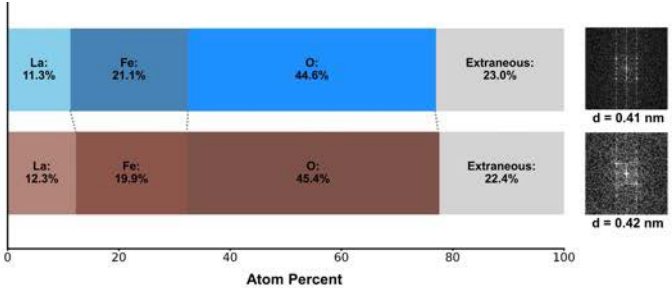
0.1 dpa Irradiation

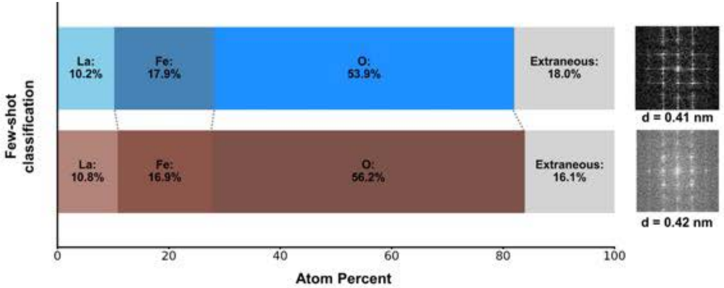


The preserved crystal regions show greater initial Fe and lower O content, pointing toward chemical drivers for disorder.

Defective







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Some key takeaways and topics for future study.

- Multimodal models can generate powerful descriptors of systems 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

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SCAN ME

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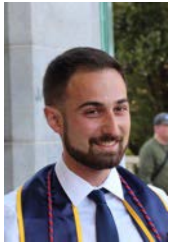

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NREL Transforming ENERGY

Multimodal models have the potential to reveal hidden materials lifecycles, transforming the design of clean energy systems.

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SCAN ME

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