NREL Transforming ENERGY

University of Colorado Boulder

From Chaos to Clarity

Autonomous Materials Discovery for Extreme Environments

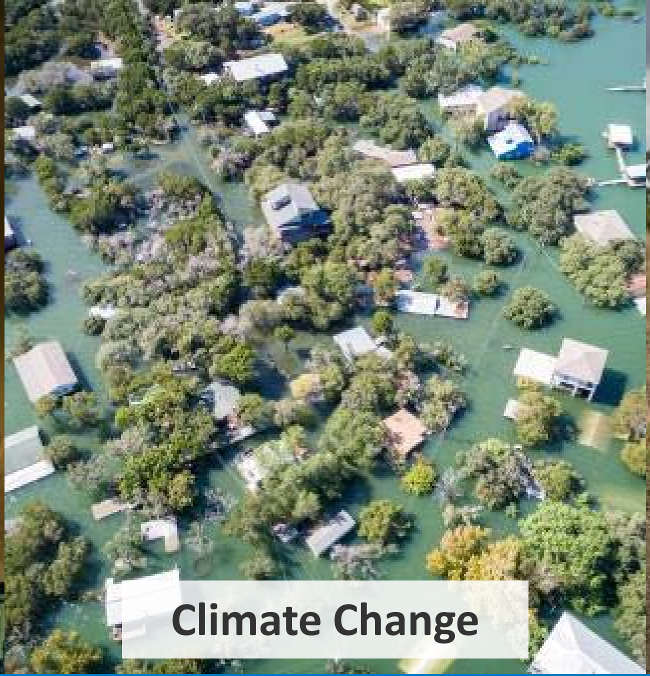
Steven R. Spurgeon

October 30, 2024

Coast to Coast

The **17** national laboratories have served as the leading institutions for scientific innovation in the United States for more than 90 years.


NREL Transforms Energy



The Triple Planetary Crisis

The **triple planetary crisis** refers to the three main issues that humanity currently faces, reinforcing one another and driving further damage. Each must be resolved for us to have a viable future on this planet.

NREL at a Glance

3,915 Workforce, including:

- 2,913 regular/limited term
- 531 contingent workers
- 223 postdoctoral researchers
- 155 graduate student interns
- 93 undergraduate student interns

—as of 5/15/2024

World-class research expertise in:

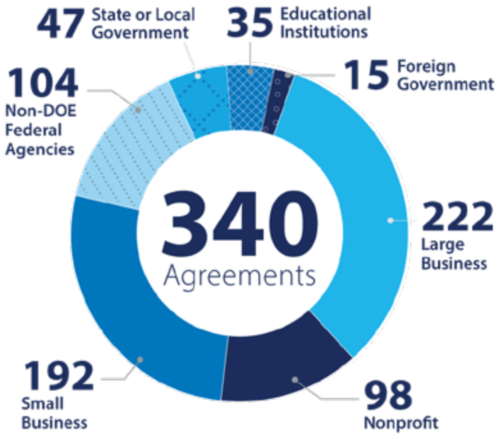
- Renewable Energy
- Sustainable Transportation & Fuels
- Buildings and Industry
- Energy Systems Integration

Partnerships with:

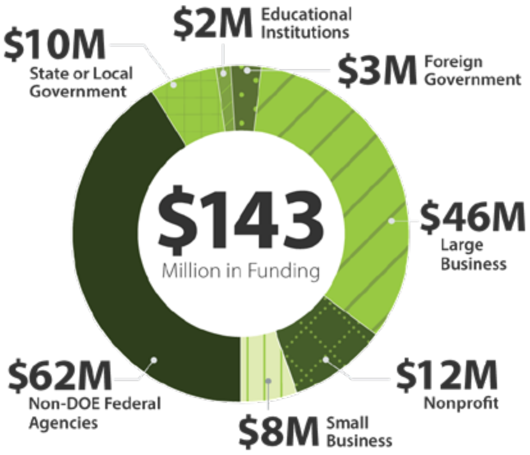
- Industry
- Academia
- Government

4 Campuses operate as living laboratories

More Than 1,100 Active Partnerships in FY 2023



Agreements by Business Type



Funding by Business Type

Integrated Energy Pathways

Electrons to Molecules

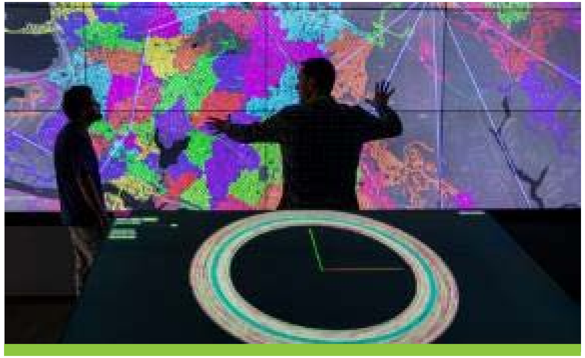
Circular Economy for Energy Materials

NREL's Vision:

A Clean Energy Future for the World

Three critical research areas respond to today's energy challenges and provide tomorrow's solutions

Integrated Energy Pathways

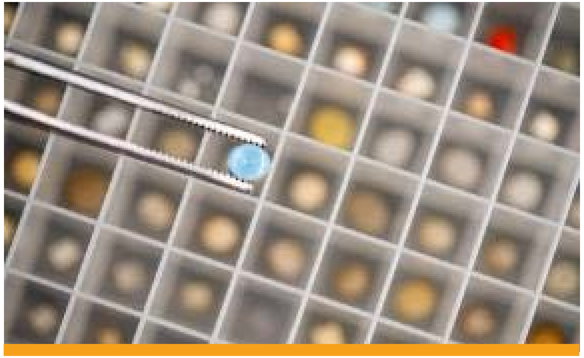


Developing the foundational knowledge and technologies to **optimize the integration of renewables, buildings, industry, energy storage, and transportation**—modernizing our energy systems and ensuring a secure and resilient grid.

Electrons to Molecules

Accelerating the **conversion of electricity and small waste gases** (e.g., CO_2, H_2O, N_2) into chemical bonds for the purposes of chemical, material, or fuel synthesis and/or energy storage.

Circular Economy for Energy Materials



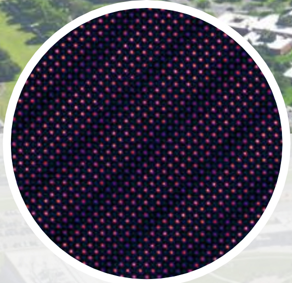
Establishing the **foundational knowledge/technology** for design, recycle, reuse, remanufacture, and reliability for **energy-relevant** materials and processes.

NREL’s Three Critical Objectives

Carnegie Mellon → Drexel → PNNL → NREL / CU

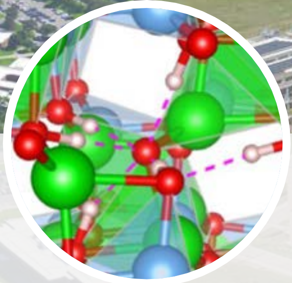
Thin Film Synthesis

Enabling devices for electronics, computing, and energy



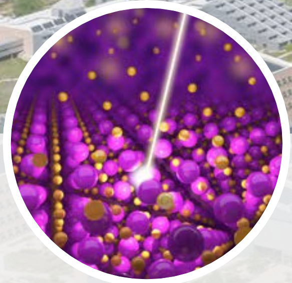
Atomic-Scale Microscopy

Understanding the fundamental building blocks of matter



Defect Engineering

Quantifying and harnessing property-defining defects



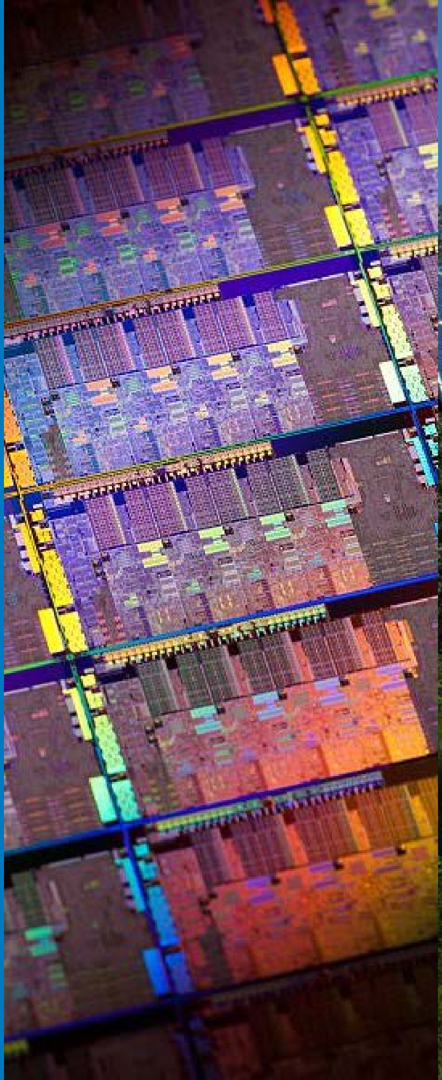
Degradation Pathways

Charting evolution in real-world extreme environments

Autonomous Science

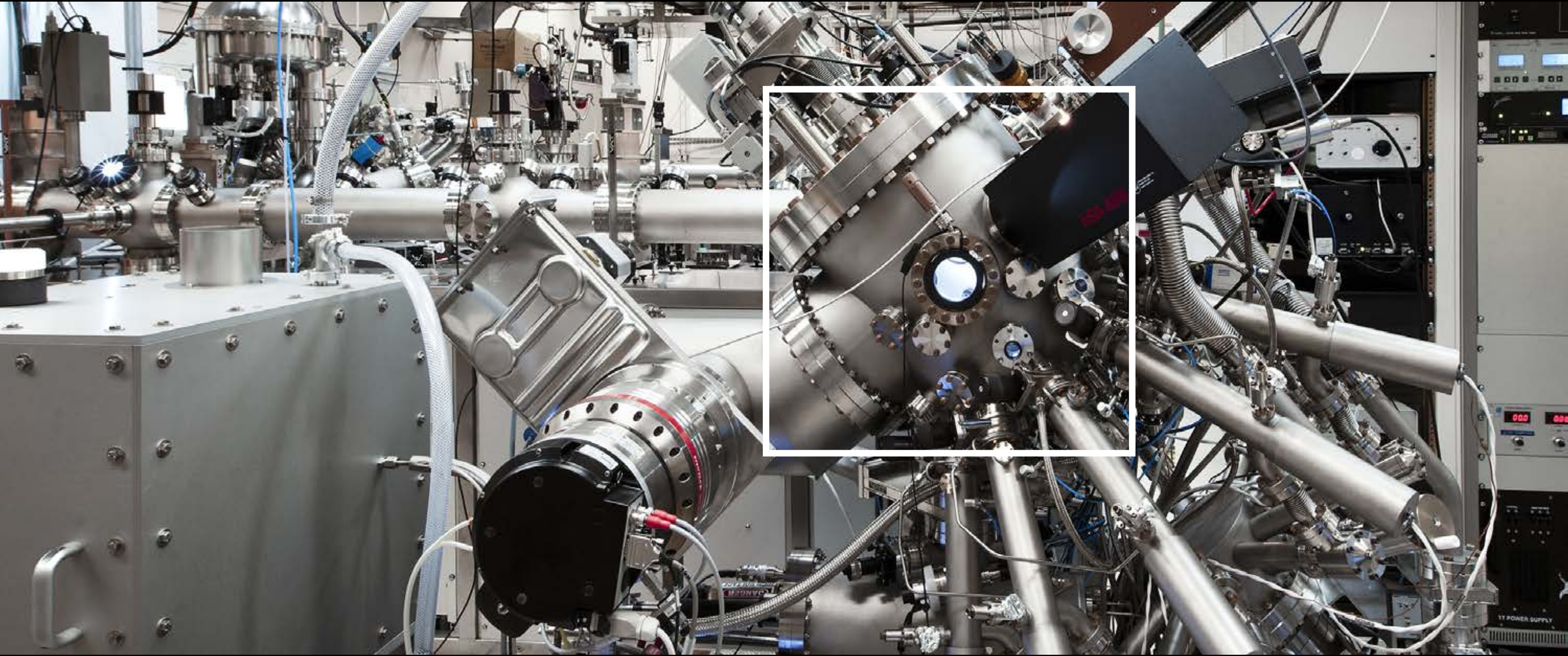
AI-accelerated materials discovery and design

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…



Oxide Epitaxy Lab @ PNNL

Mastery depends on understanding of complex synthesis pathways…

Kaganer. Paul Drude Institute.

…and degradation behavior in real-world extreme environments.

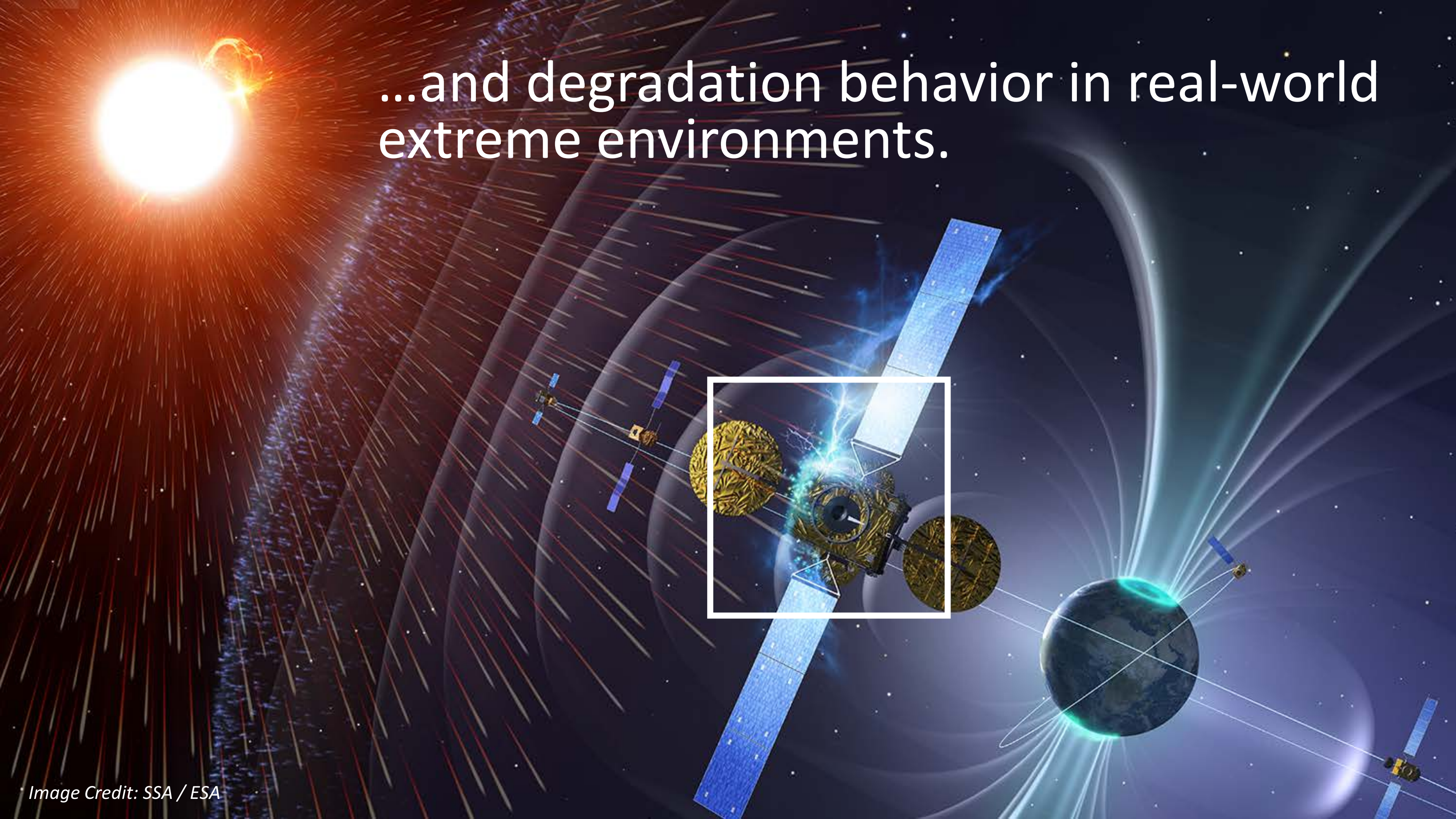
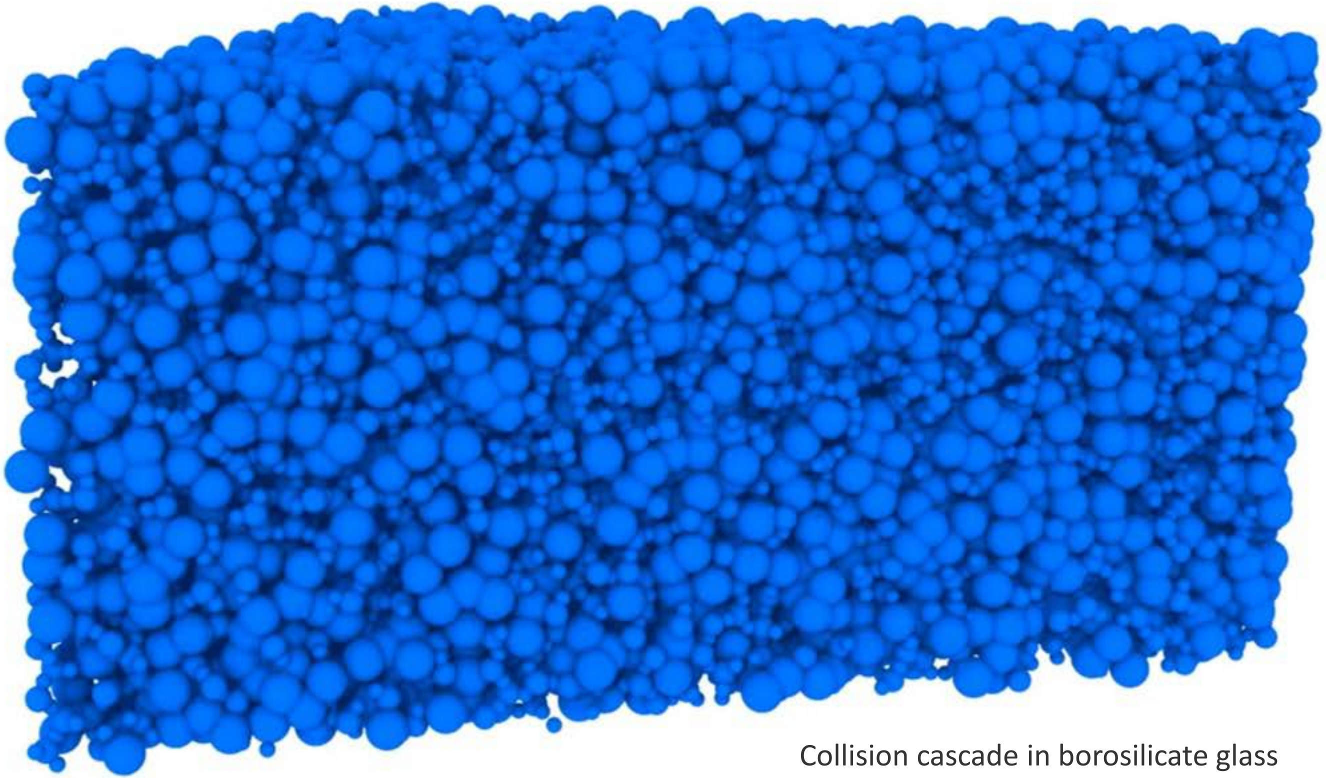


Image Credit: SSA / ESA

…and degradation behavior in real-world extreme environments.

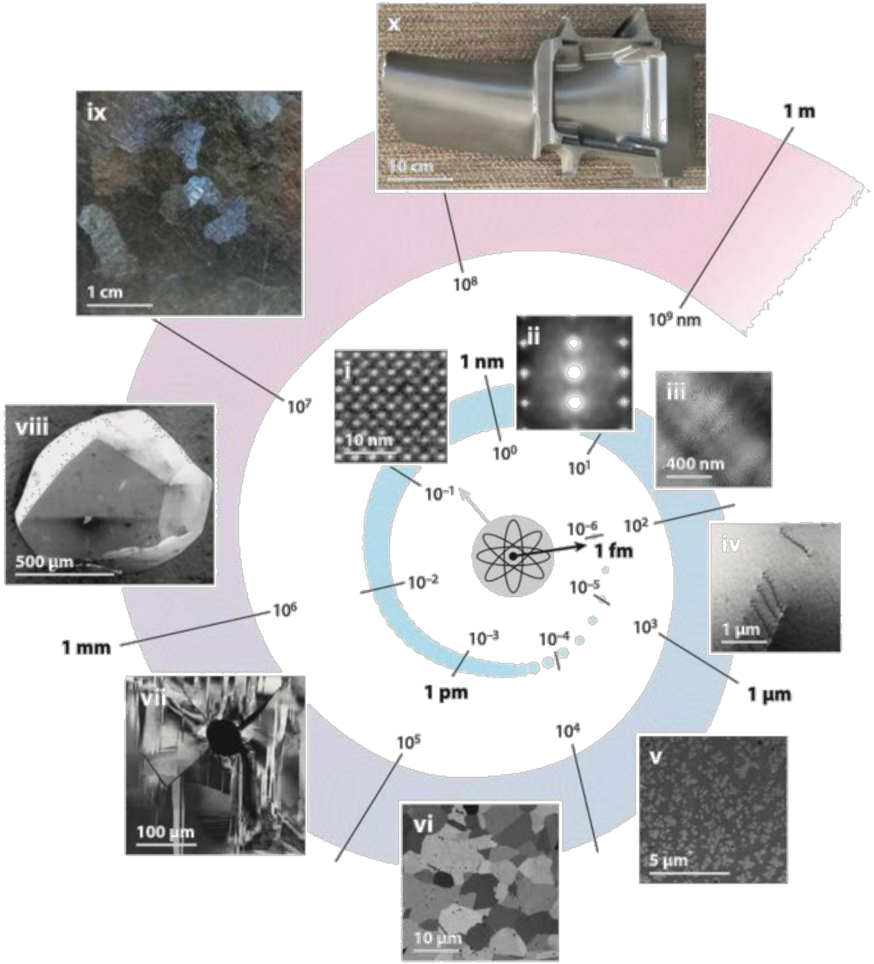


Collision cascade in borosilicate glass

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

My research aim is an ontology of the materials lifecycle:

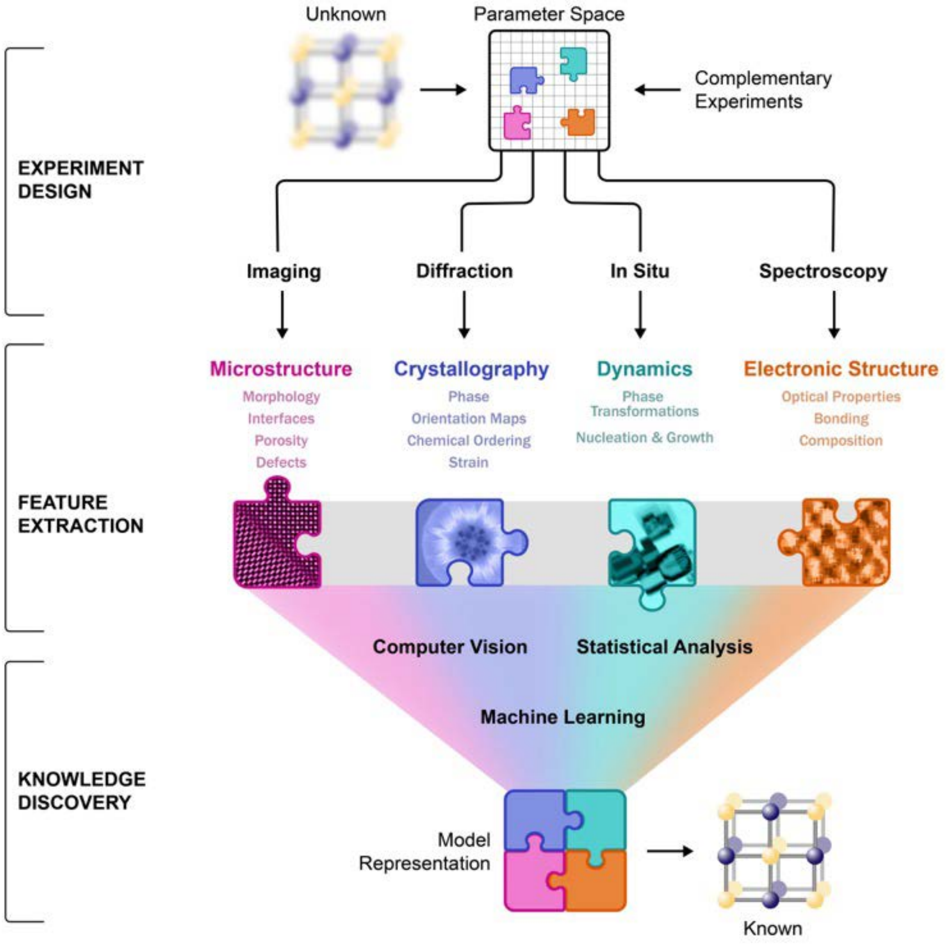
*"A systematic mapping of data to meaningful semantic concepts…" **across spatial and temporal scales***



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

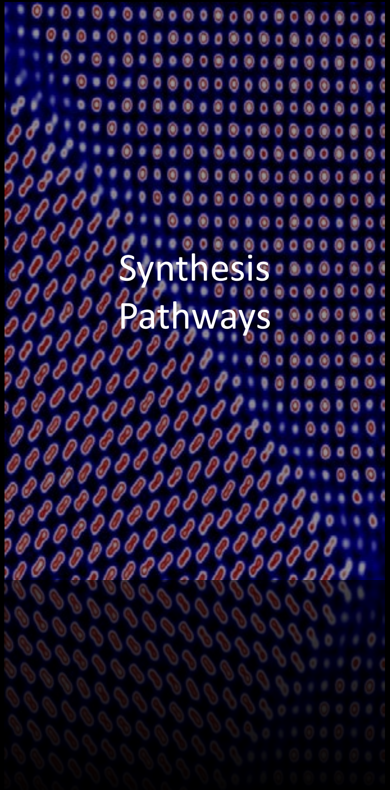
Quote adapted from: https://blog.palantir.com/ontology-finding-meaning-in-data-palantir-rfx-blog-series-1-399bd1a5971b

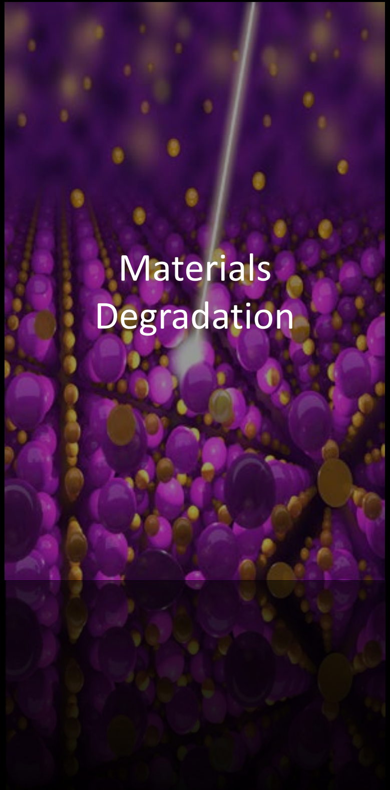
Autonomous science plays an important role in developing and harnessing this ontology

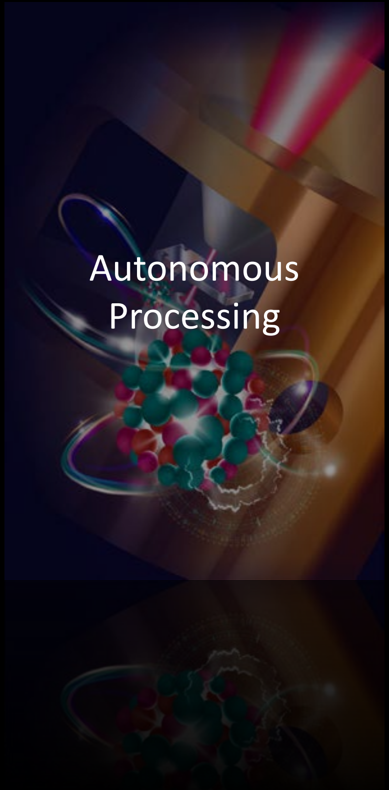


Spurgeon et al. Nature Mater, 20(3), 274–279. (2021).

Today I'll discuss accelerating materials design through autonomous science in three areas







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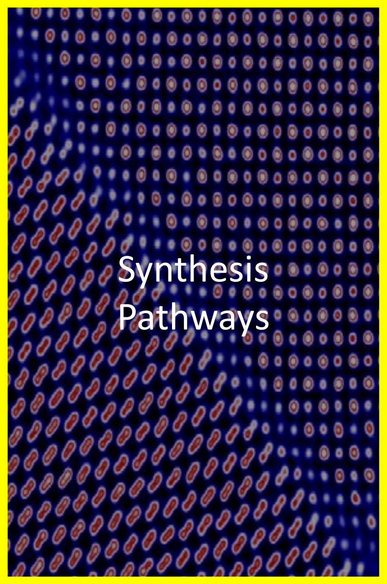
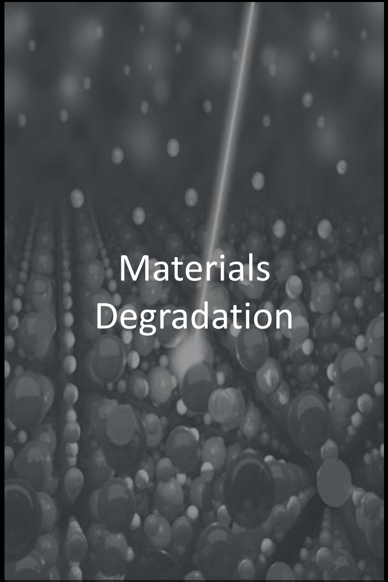
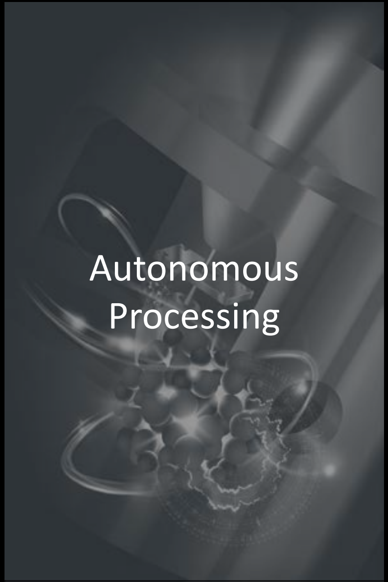
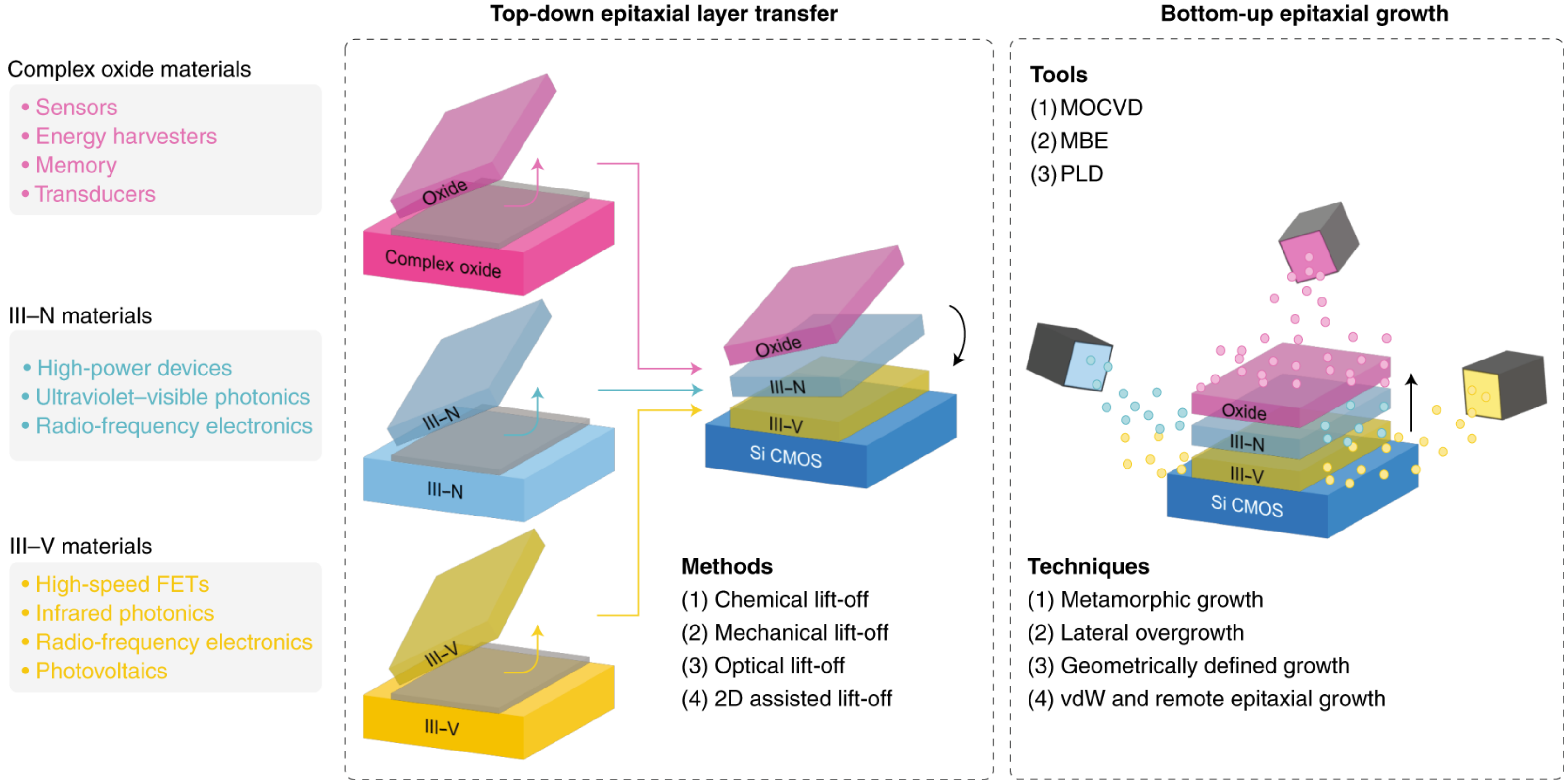






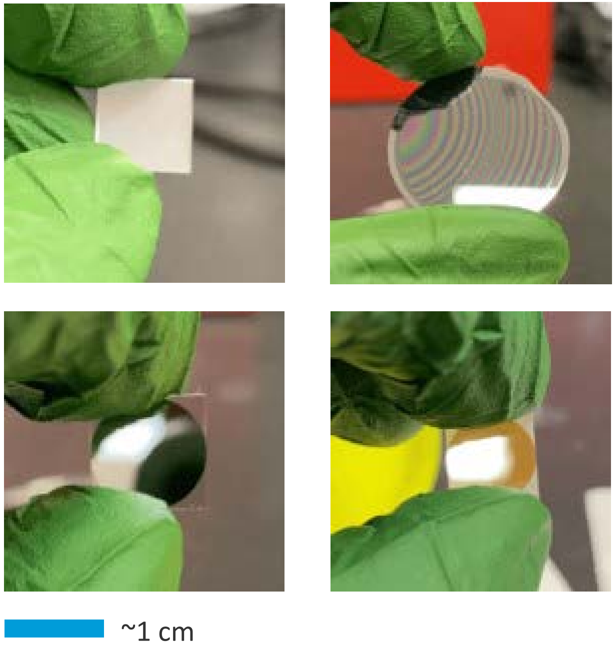
Epitaxial integration of semiconductors and oxides is a challenge for emerging devices

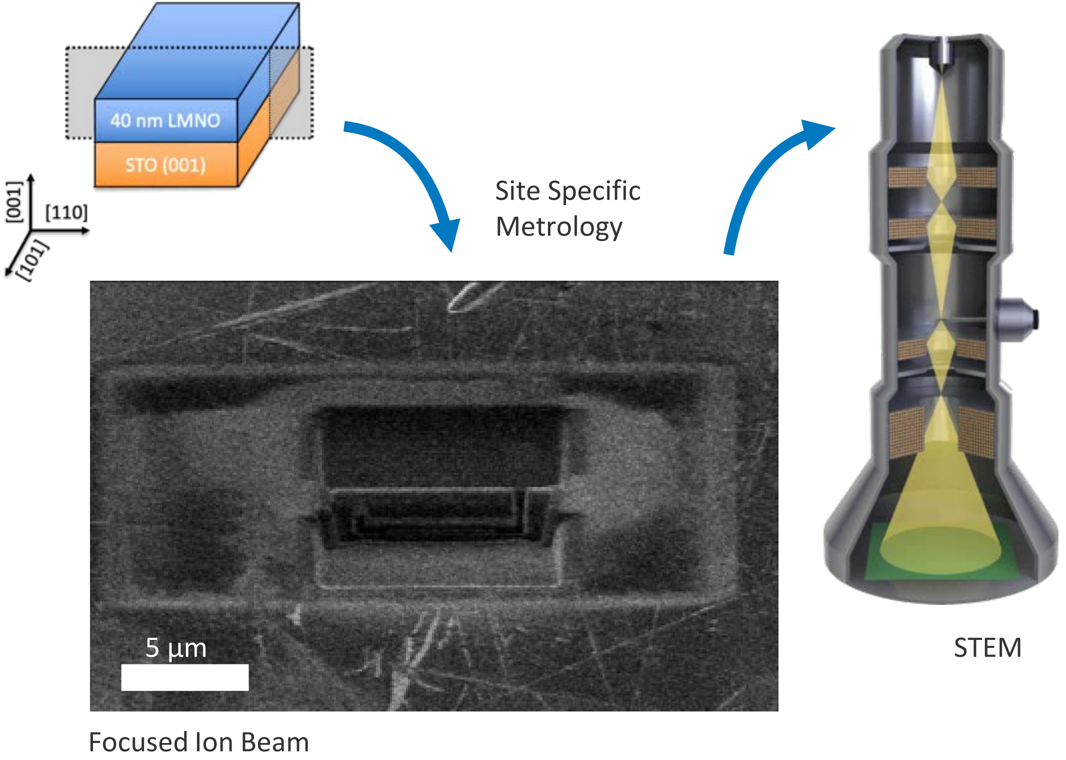


Kum et al. Nature Electron. 2, 439–450 (2019).

Tailored materials design requires direct local probes of structure and chemistry

Functional Thin Films for Energy Applications

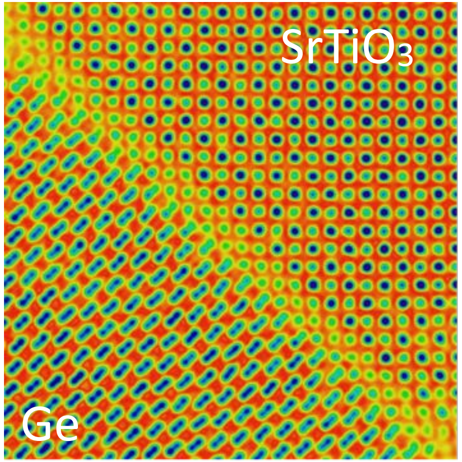




Spurgeon et al. Chem Mater, 28.11. 3814–3822. (2016).

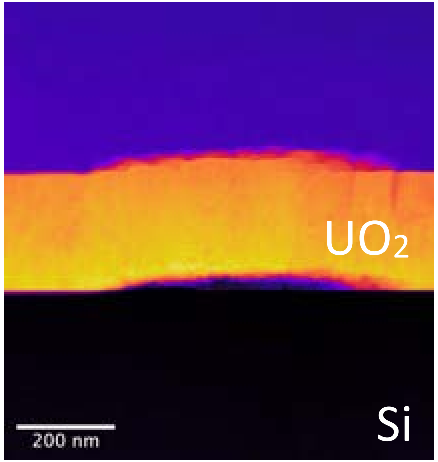
Electron microscopy can richly inform lifecycle models to achieve predictive control

Structure → **Chemistry**



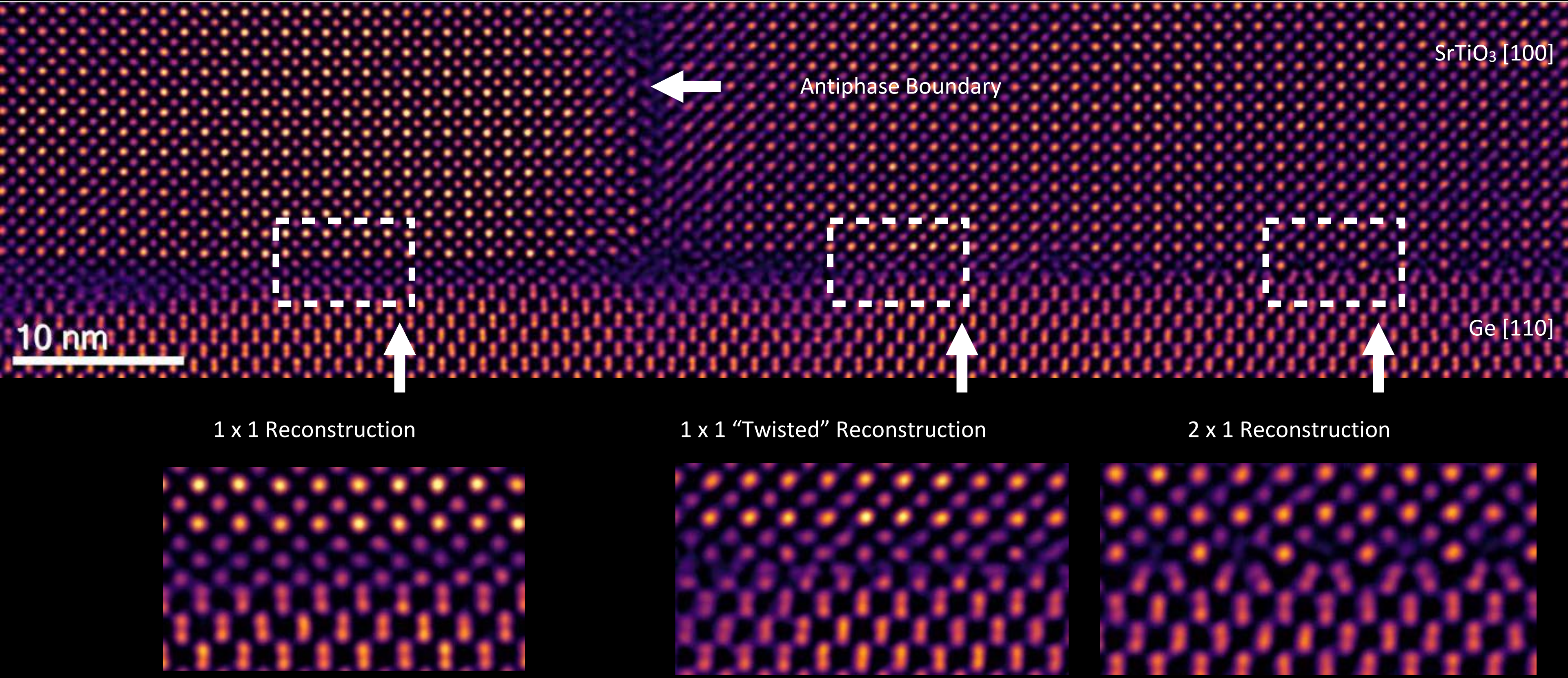
Imaging

Diffraction



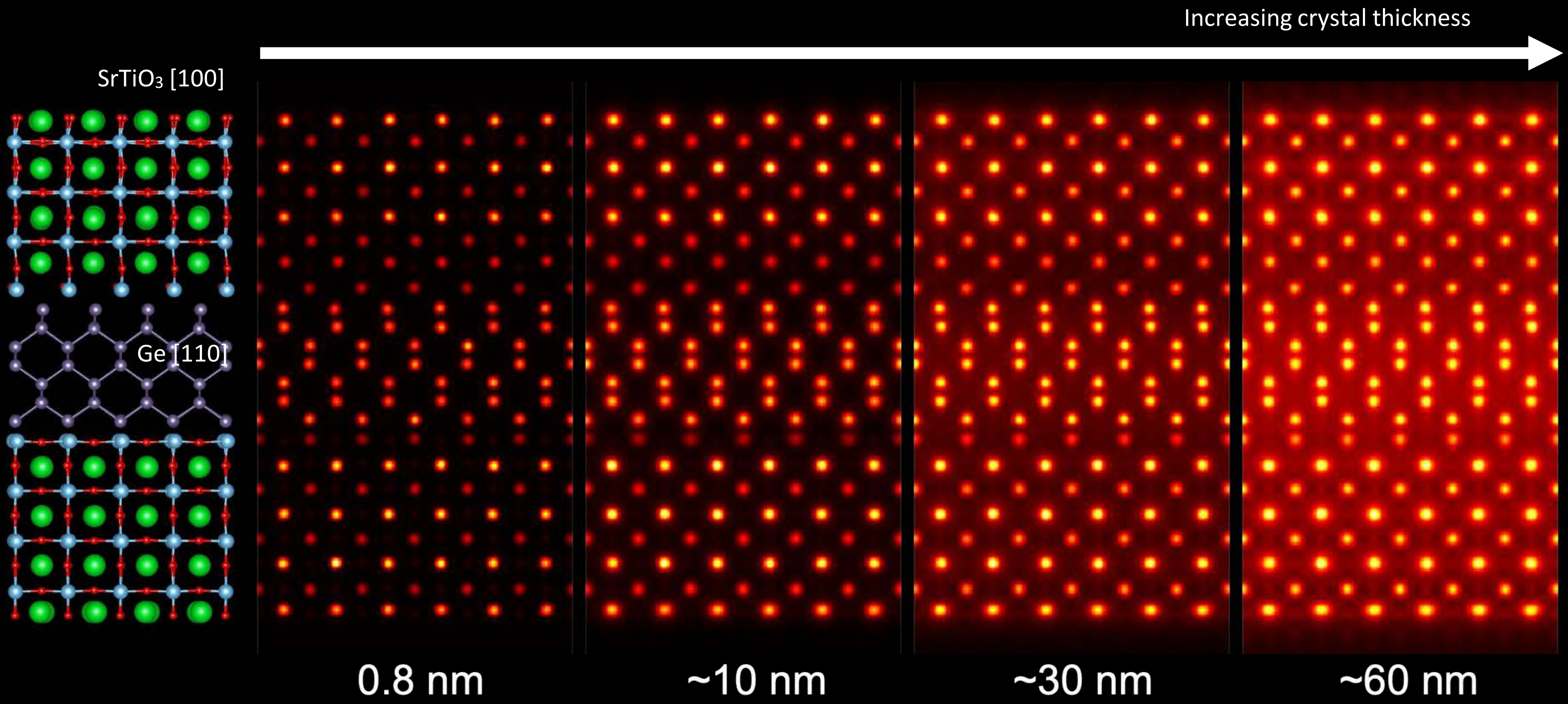
Spectroscopy

We have examined interfacial reconstructions in STO / Ge grown via low oxygen pressure MBE



Du et al. Phys Rev Mater. 2. 094602. (2018).

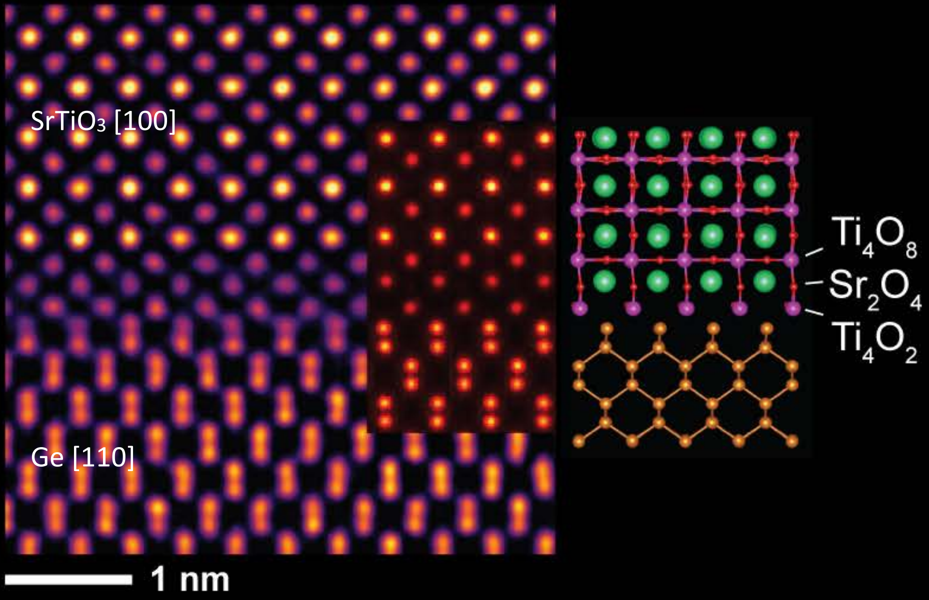
We can directly integrate DFT calculations of interface structures with microscope images



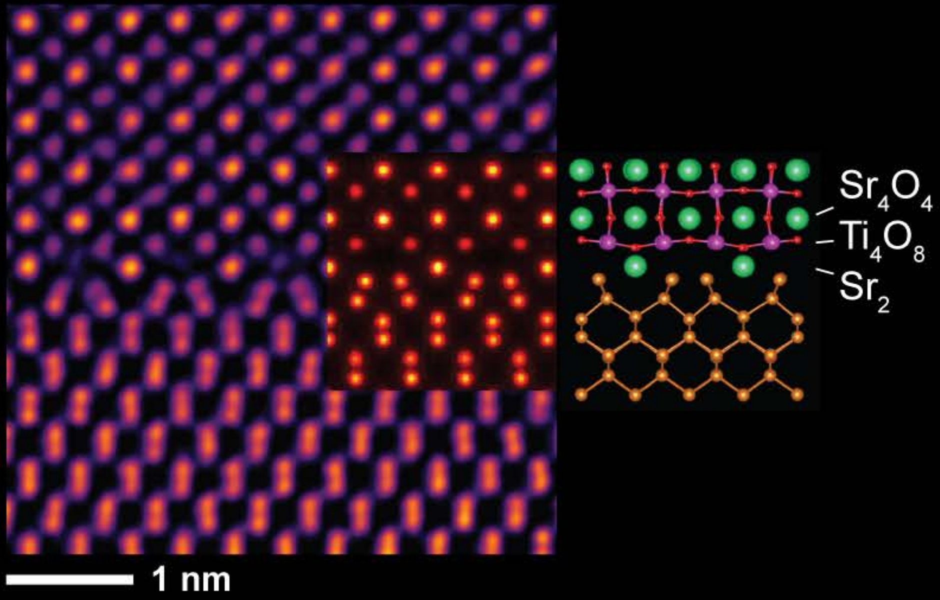
Du et al. Phys Rev Mater. 2. 094602. (2018).

This allows us to determine solutions for interface reconstruction and resulting band structure

1 x 1 Reconstruction

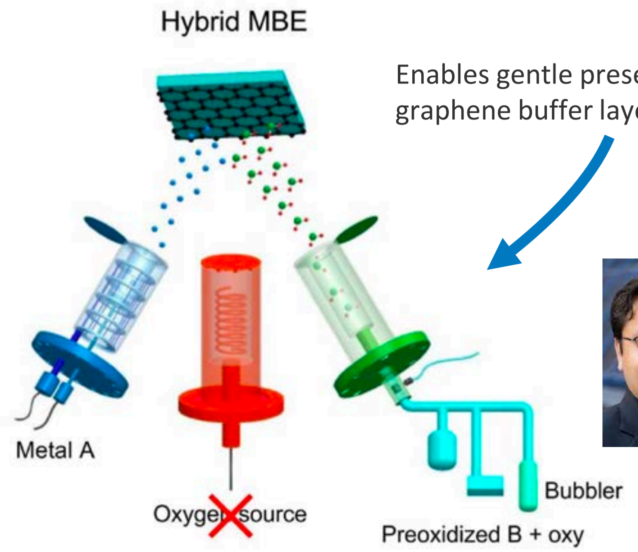


2 x 1 Reconstruction

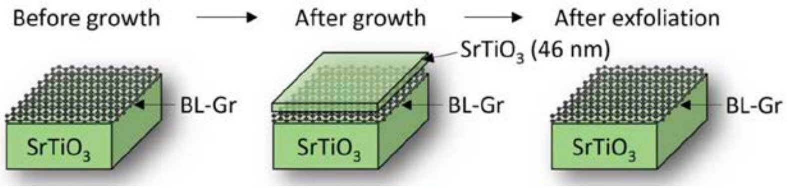


Du et al. Phys Rev Mater. 2. 094602. (2018).

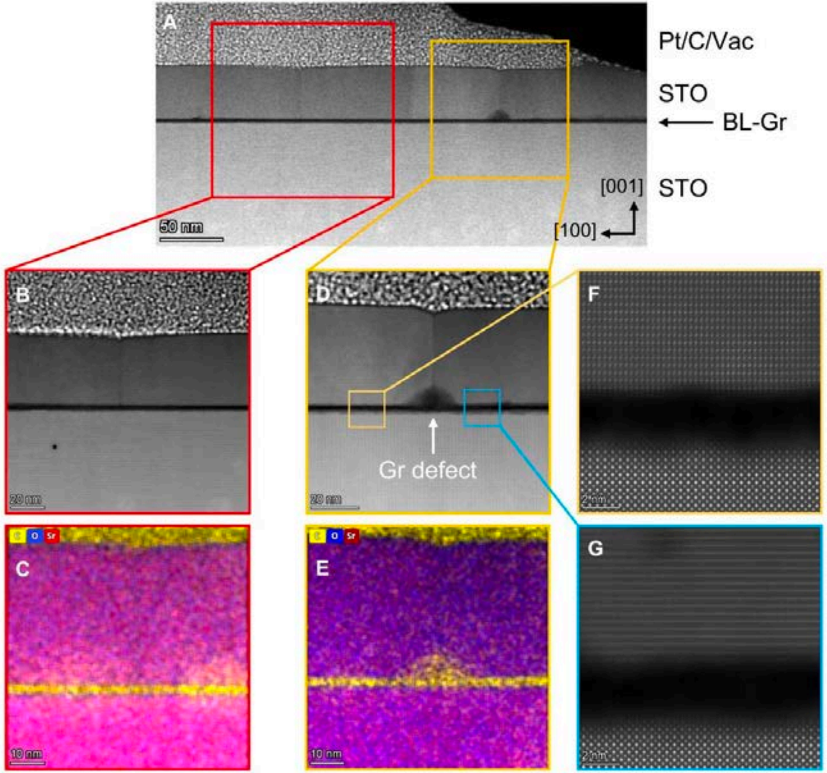
Using hybrid MBE growth, we have demonstrated successful STO lift off from buffered graphene



Enables gentle preservation of graphene buffer layers

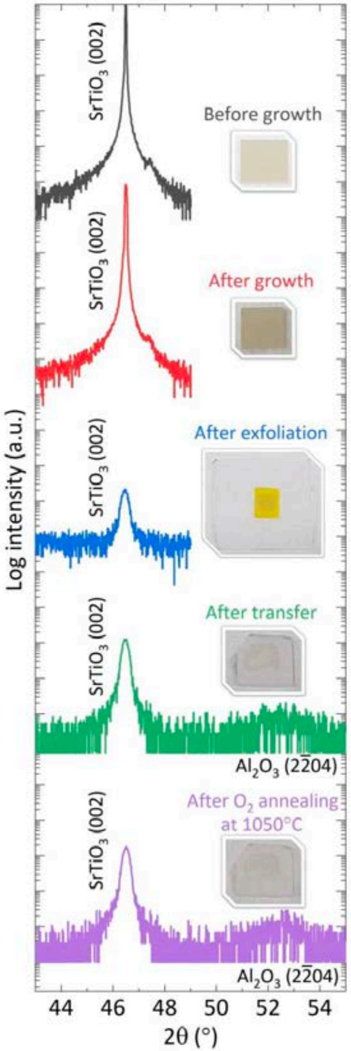


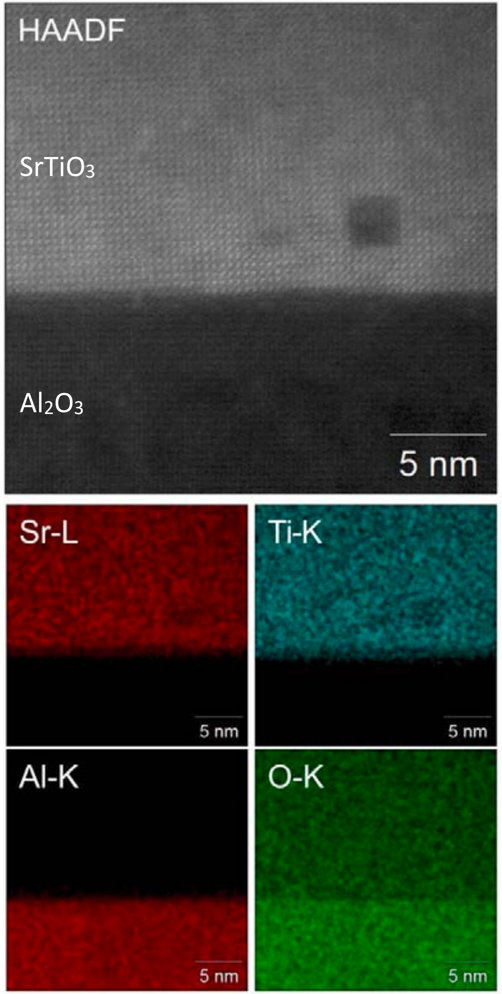
Bharat Jalan
U. Minnesota



Yoon et al. Sci Adv 8, eadd5328 (2022).

We can transfer crystalline films to foreign substrates, unlocking completely new architectures

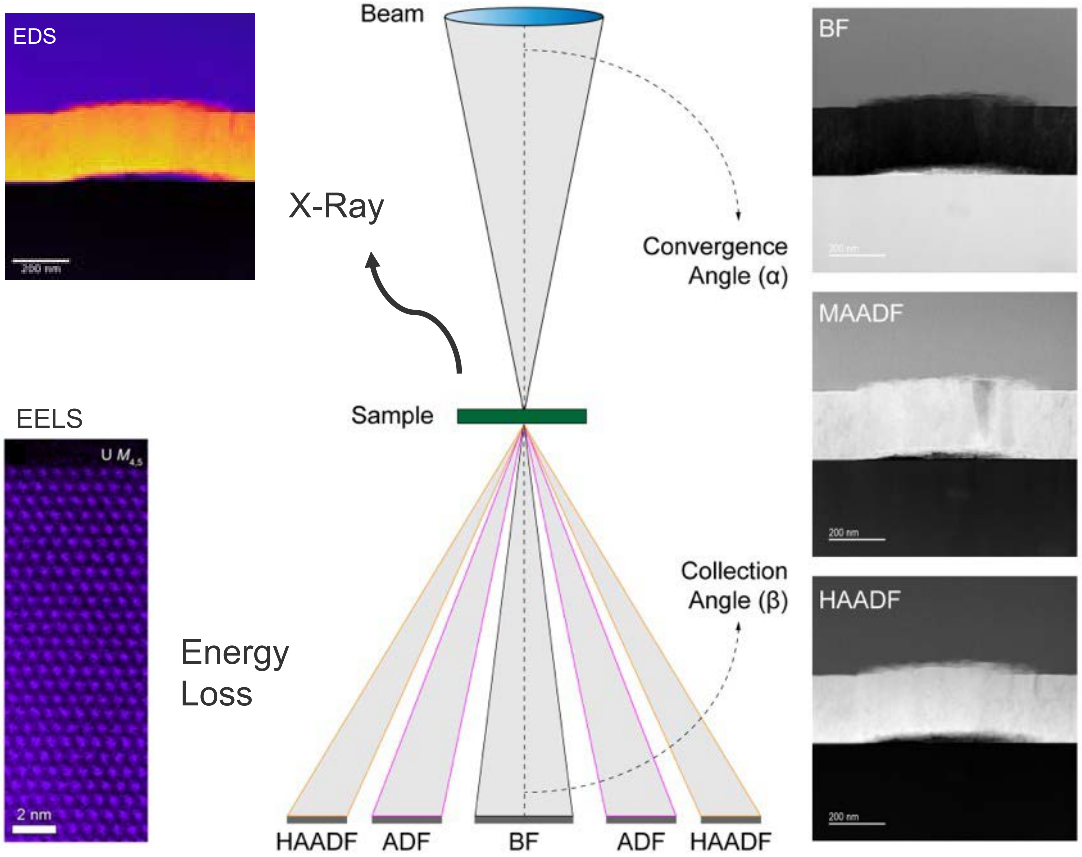




Yoon et al. Sci Adv 8, eadd5328 (2022).

The Challenge

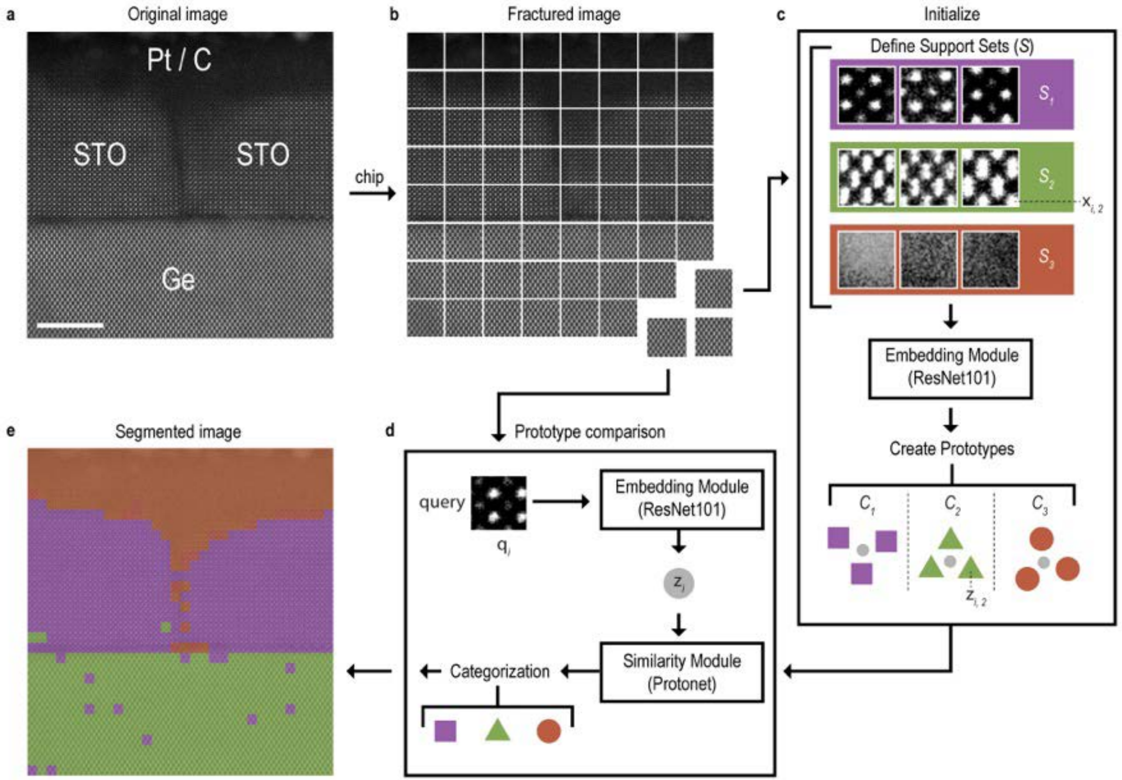
How do we move from laborious one-off “hero” experiments to truly statistical models?



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

Spurgeon et al. PNAS 116, 17181. (2019).

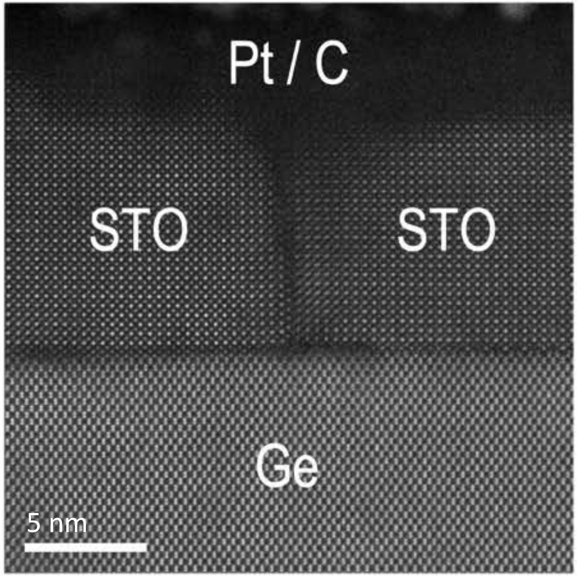
Few shot learning uses limited prior knowledge to classify features in discovery scenarios



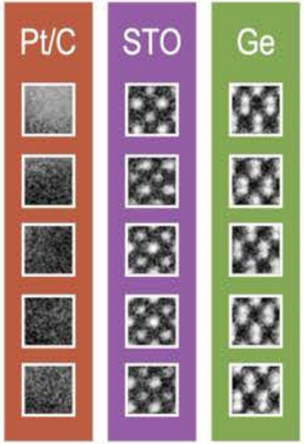
Akers et al. npj Comp. Mater., 7(1), 187. (2021).

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

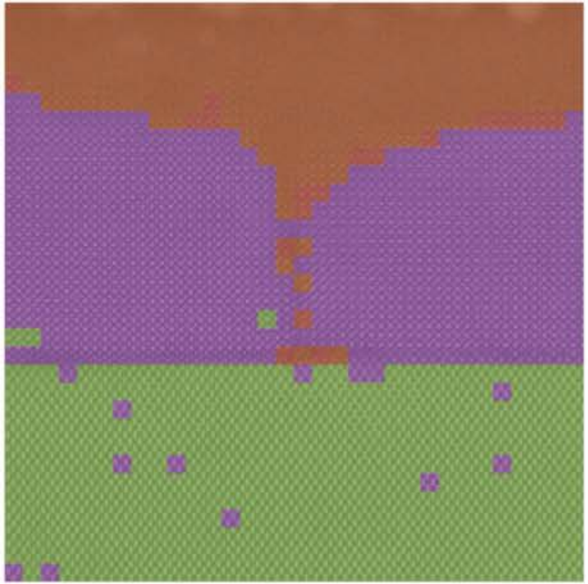
Original HAADF Image



Support Sets



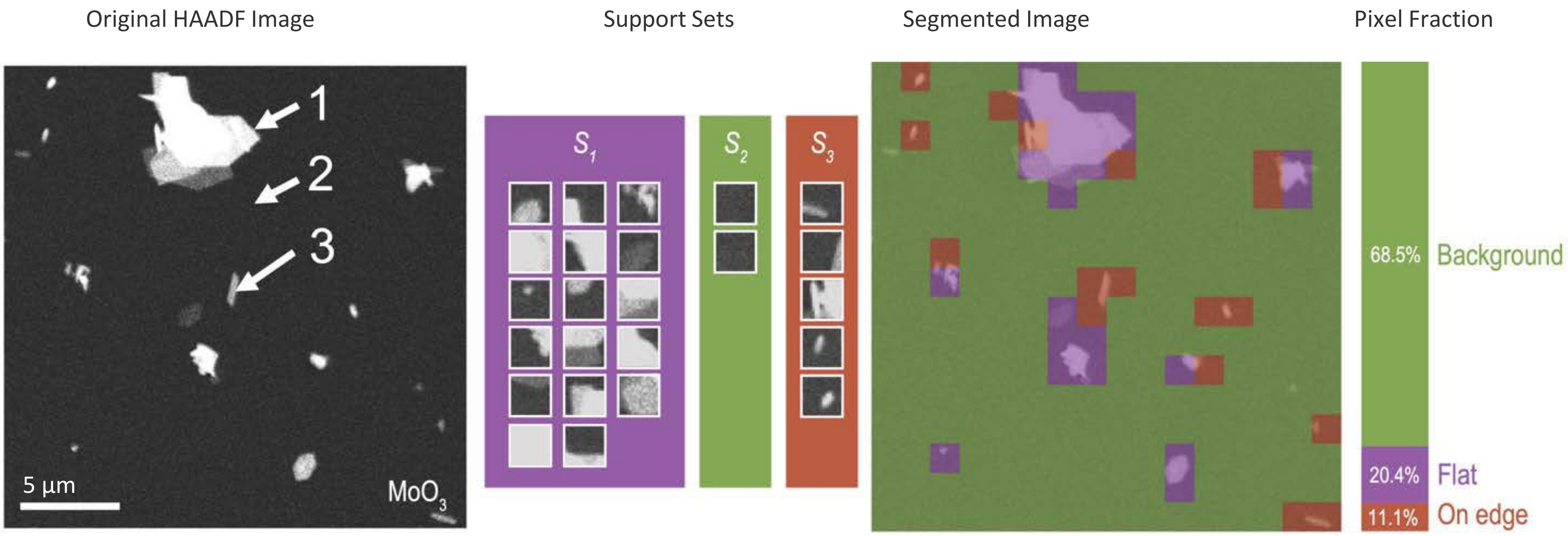
Segmented Image



Pixel Fraction

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

Such a model can easily be applied to different synthesis tasks

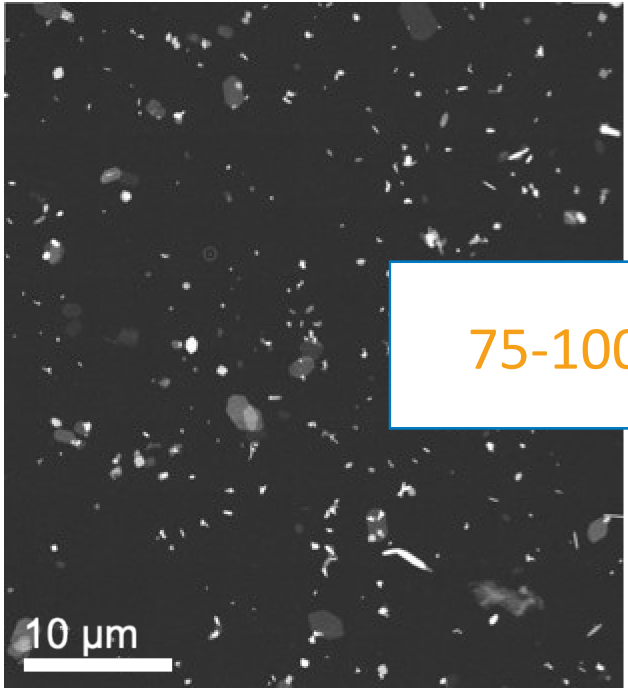


Akers et al. npj Comp. Mater., 7(1), 187. (2021).

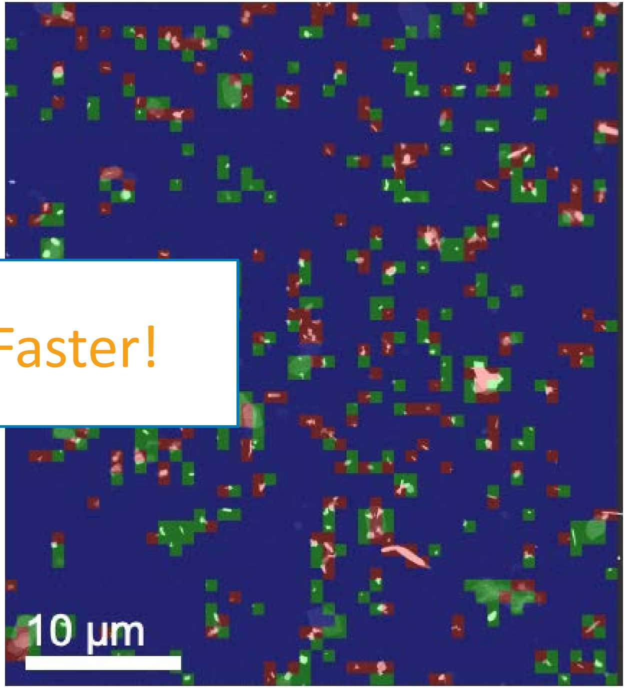
We can ultimately extract materials descriptors in a faster and more reproducible manner

MoO_3

Manual Analysis
10 minutes



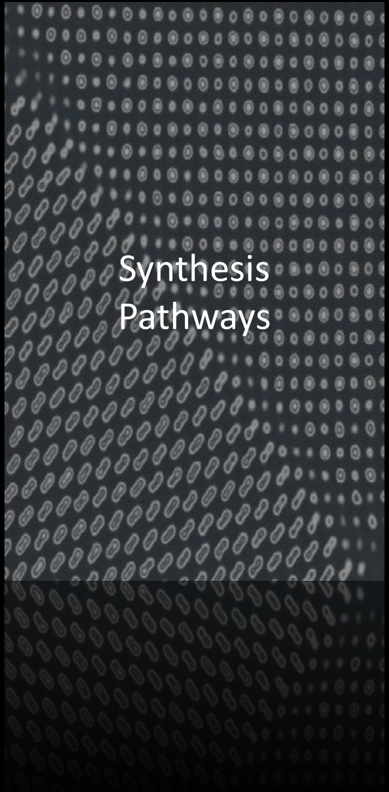
75-100x Faster!

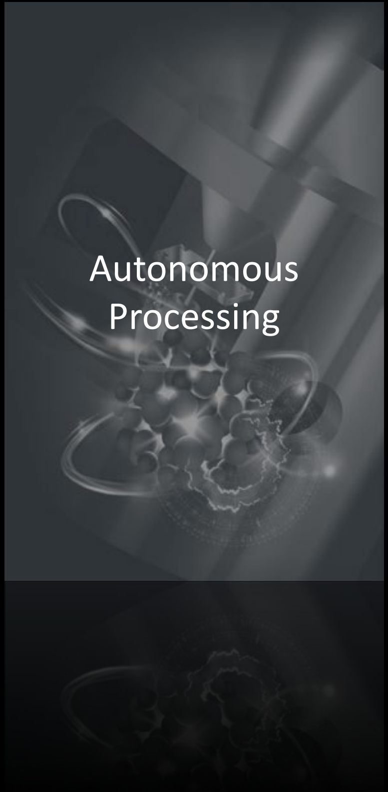


Few-Shot
Task 2
8 seconds

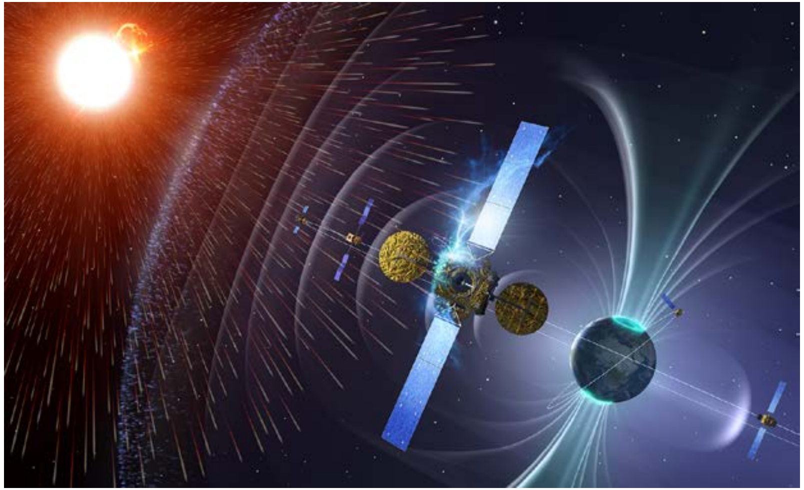
Akers et al. npj Comp. Mater., 7(1), 187. (2021).

Today I'll discuss accelerating materials design through autonomous science in three areas

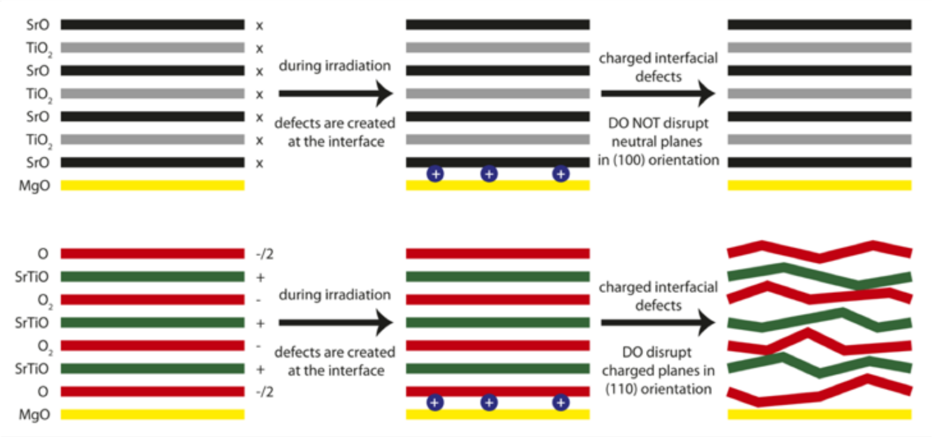




Controlling materials degradation is critical for electronics and sensors in extremes

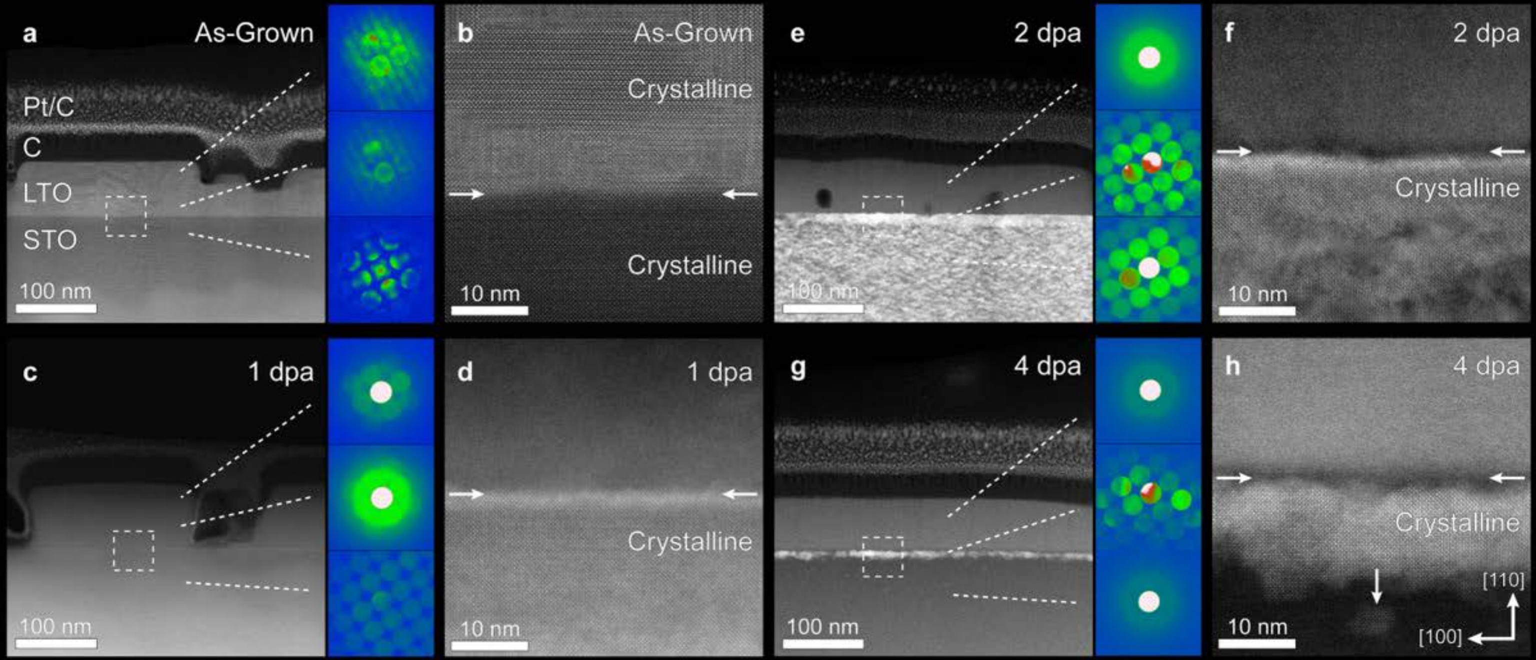


How does interface configuration affect radiation-induced disorder in devices?



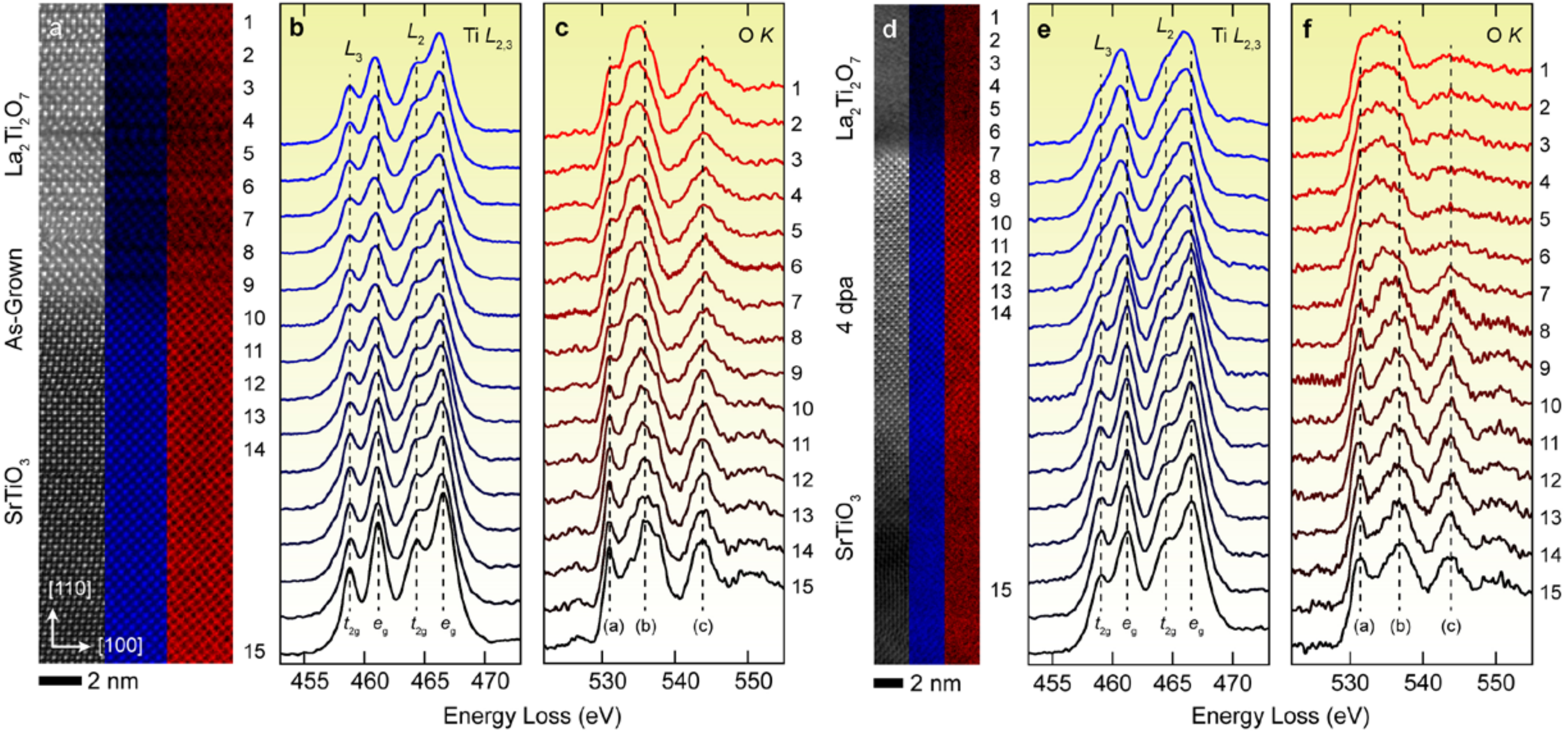
Aguiar et al. J. Mater. Res. 29(16), 1699–1710 (2014). | Spurgeon. Curr. Opin. Solid. State Mater. Sci. 24(6), 100870 (2020). | Image: SSA / ESA

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



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

Atomic-scale spectroscopy reveals changes in oxygen vacancies upon irradiation

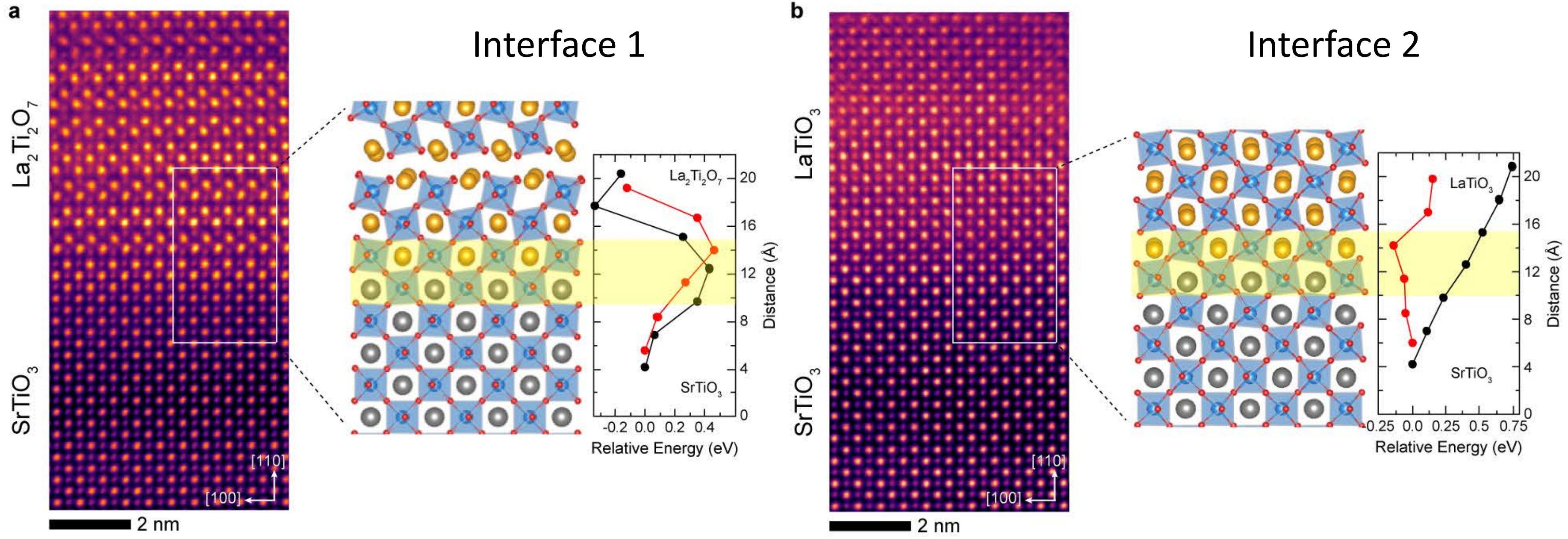


Spurgeon et al. Adv. Mater. Interfaces. 7(8). 1901901944. (2020).

This informs DFT calculations, which show differences in oxygen vacancy formation energy

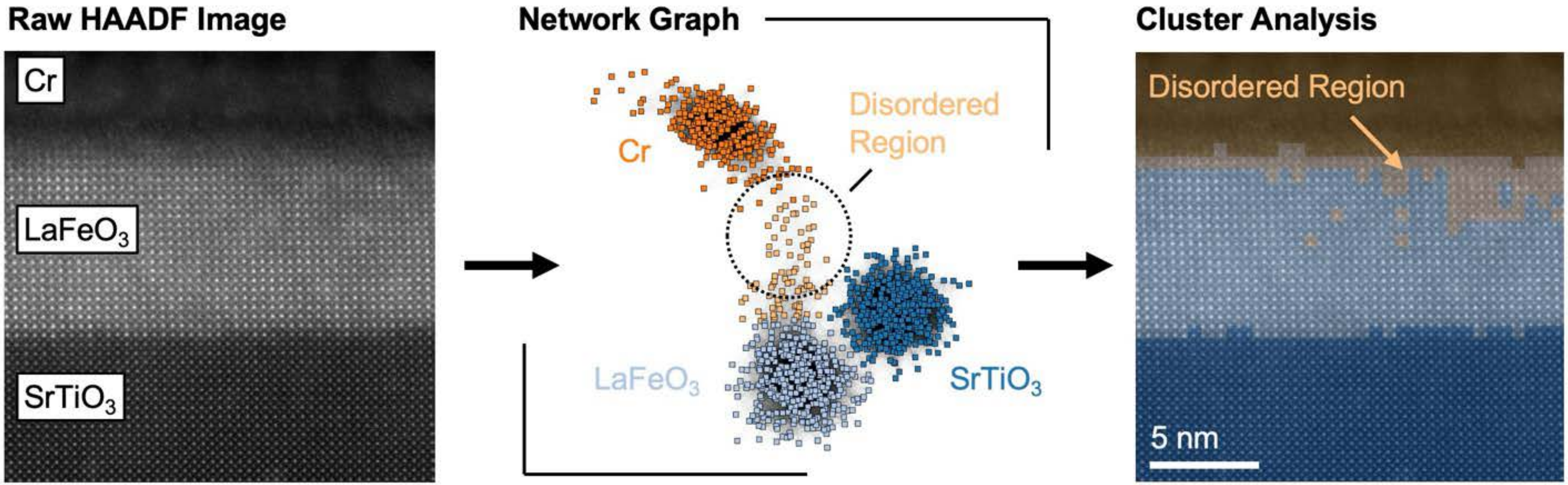
Interface 1

Interface 2



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

But how do we begin to move toward more statistical models of defects?



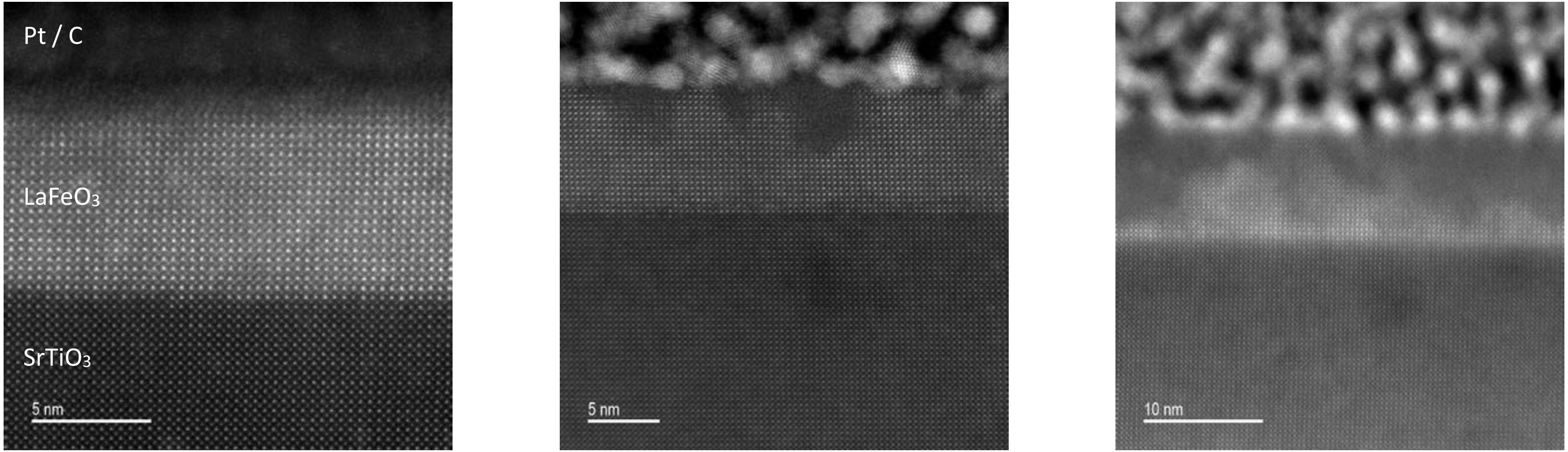
Ter-Petrosyan et al. Proc. Thirty-Seventh Conf. on Neural Information Processing Systems (NeurIPS). (2023). DOI:10.48550/arXiv.2311.08585

These descriptors help us evaluate degradation during irradiation in an unsupervised manner

0 dpa

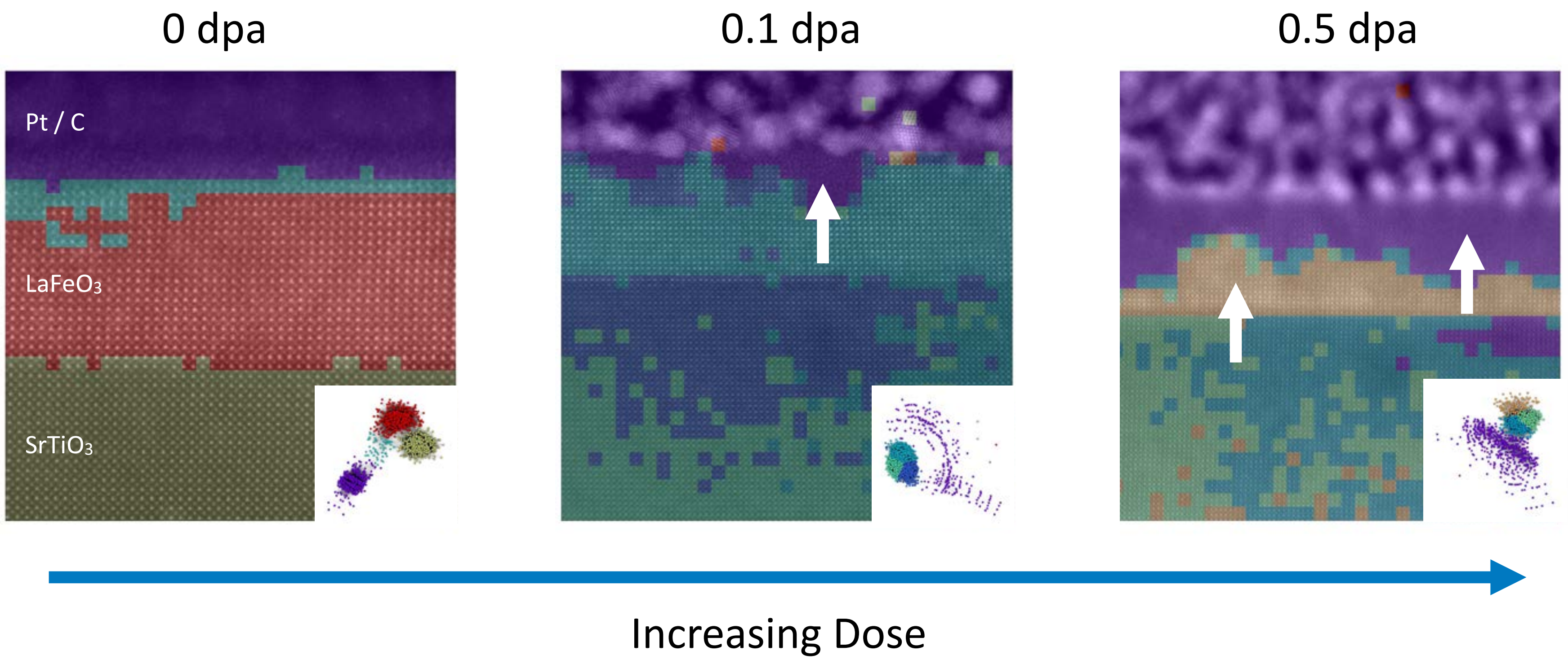
0.1 dpa

0.5 dpa



Increasing Dose

The signature of radiation damage can be tracked and used to guide next steps of synthesis



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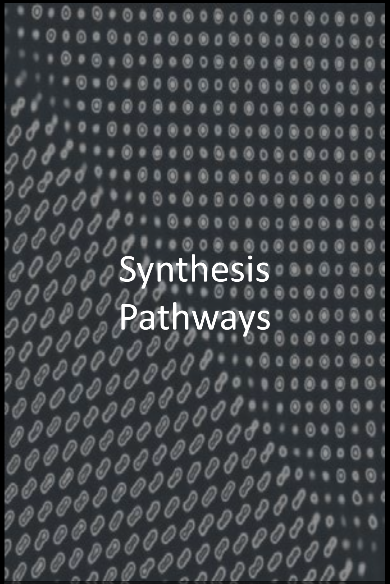
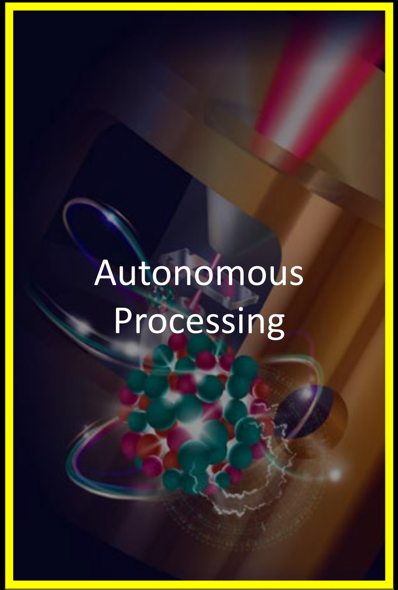
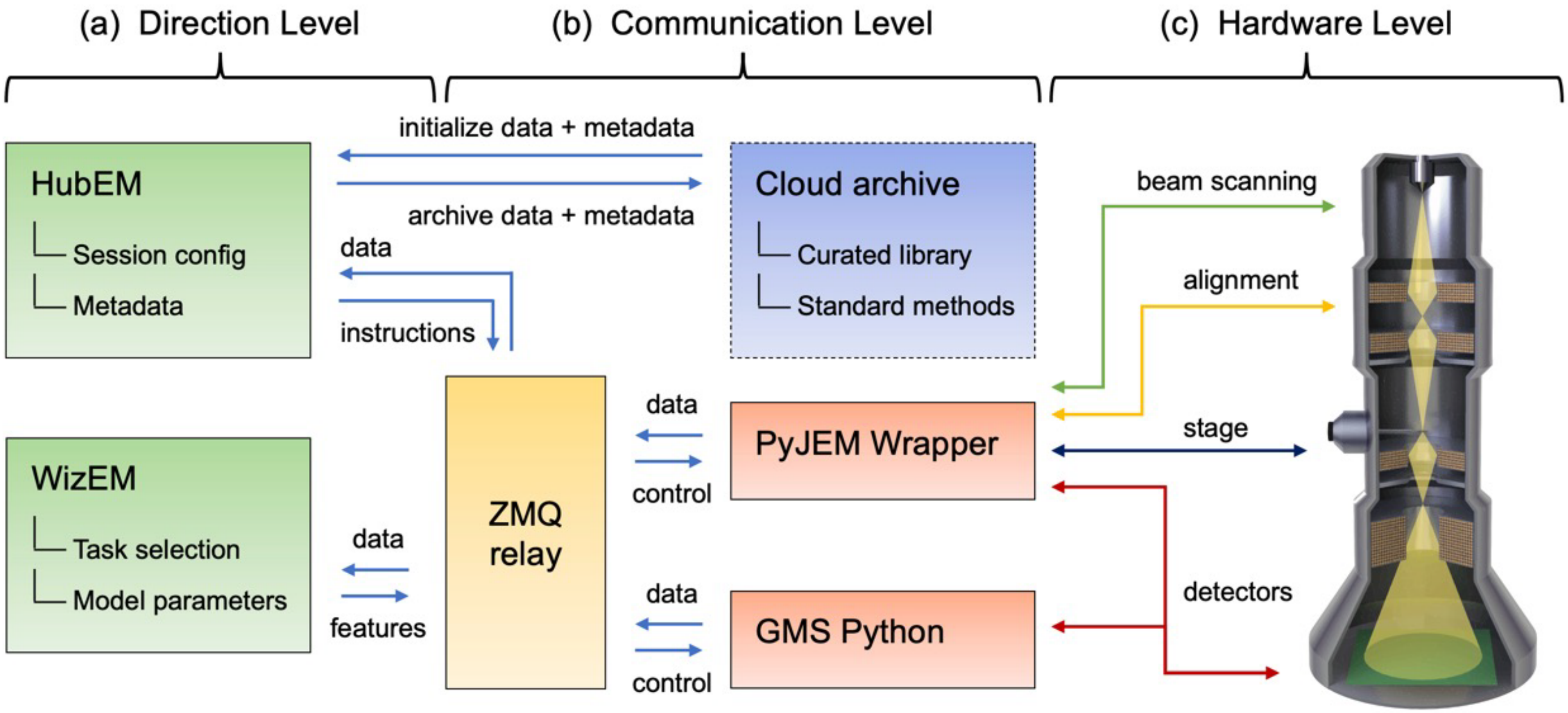


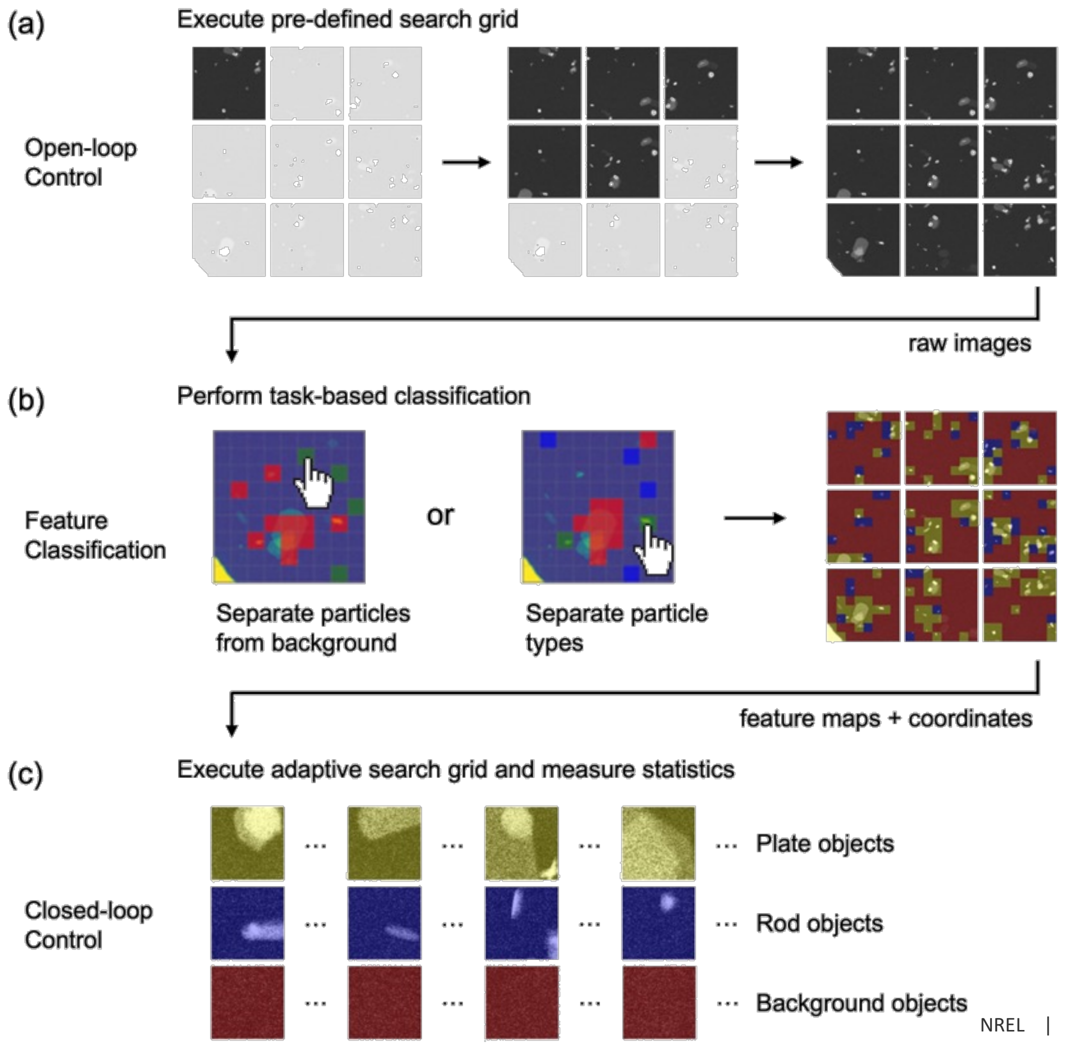


How to we embed AI control into our instruments to not just describe defects, but to impart them?



Olszta et al. Micro. Microanal., 28 (5), 1611-1621. (2022).

This platform enables intelligent closed-loop experiments and statistical analyses

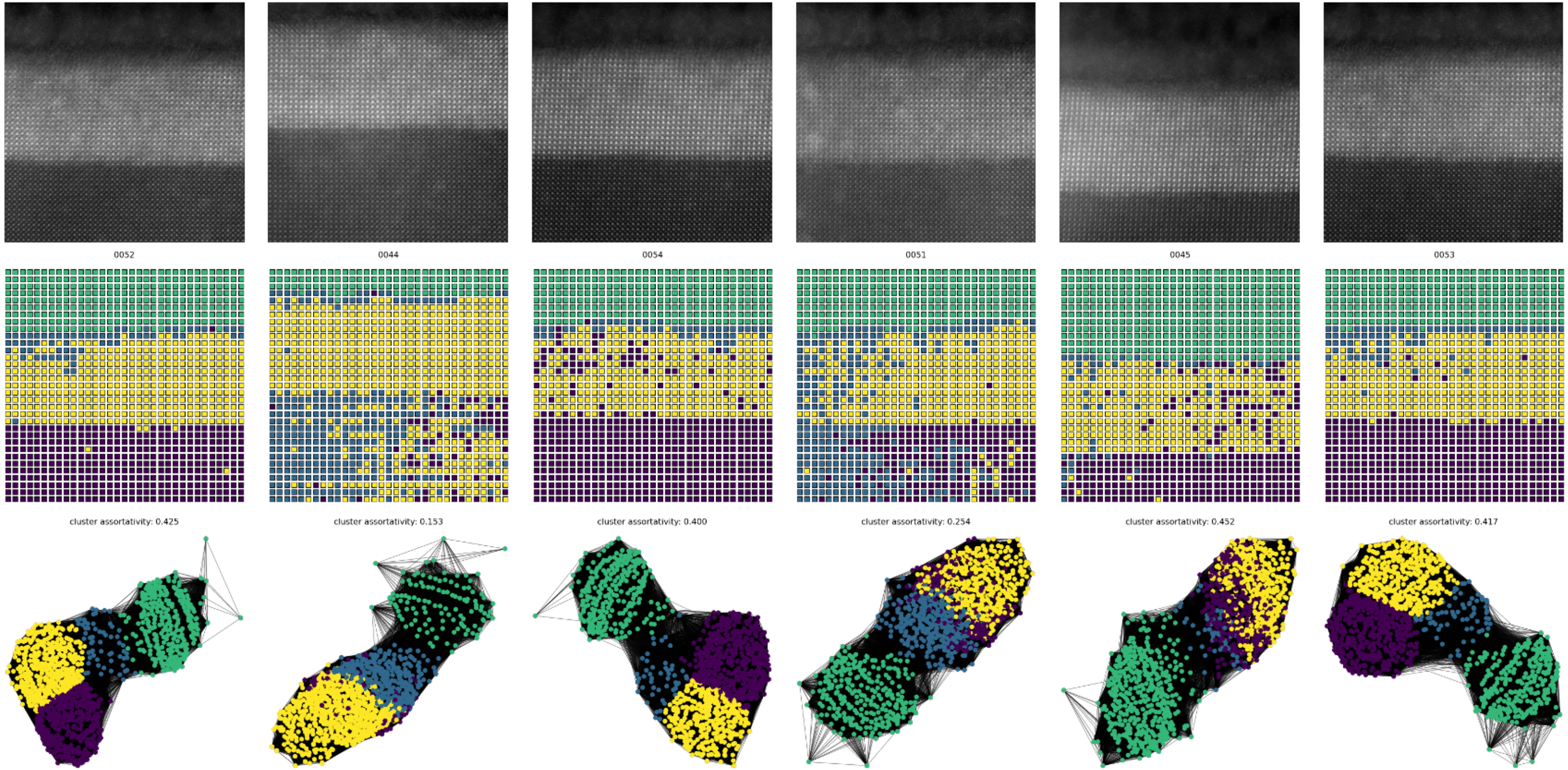


Olszta et al. Micro. Microanal., 28 (5), 1611-1621. (2022).

2024 R&D 100 WINNER

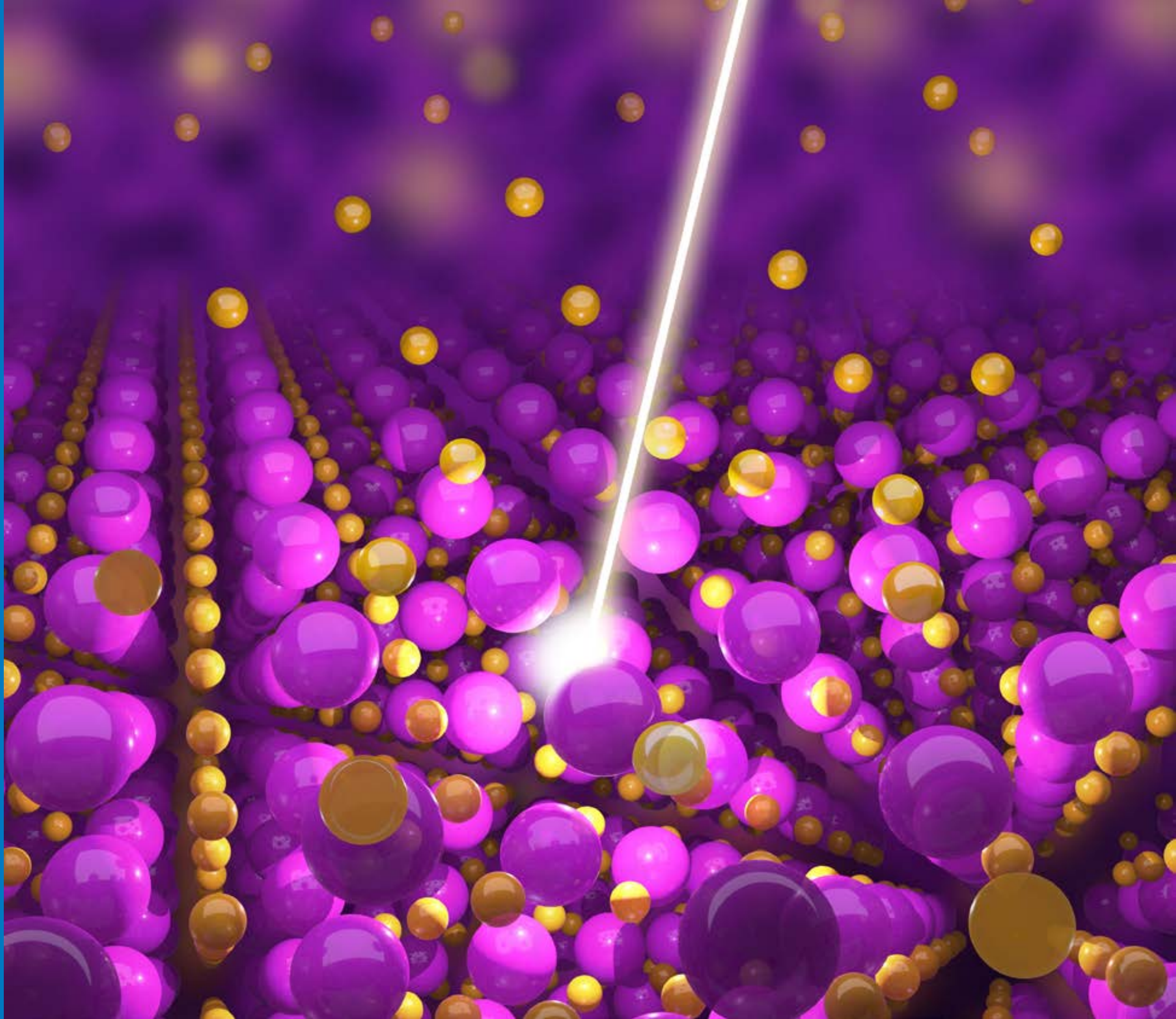
PATENT PENDING
HTTPS://YOUTU.BE/XKYJ1UAE6JE

We can build statistical libraries of synthesis and degradation products



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

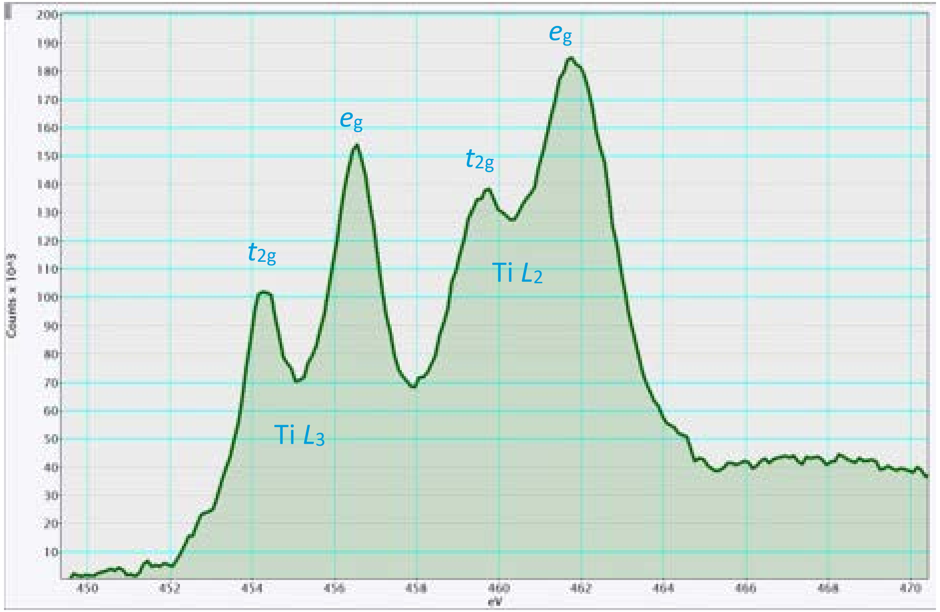
Taking this a step further, can we intelligently process materials?



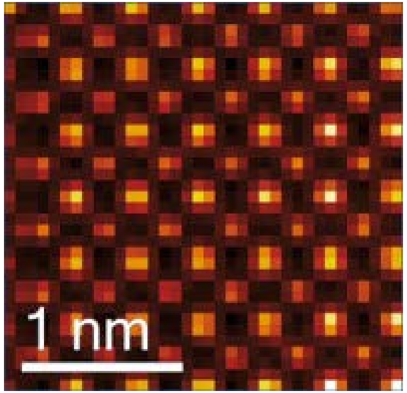
We can controllably run reactions in our microscope to impart specific defect configurations

In Situ Reduction of STO
Dose Rate ~10^9 e / (Å^2 • s)
Temp ~20 ºC

EELS

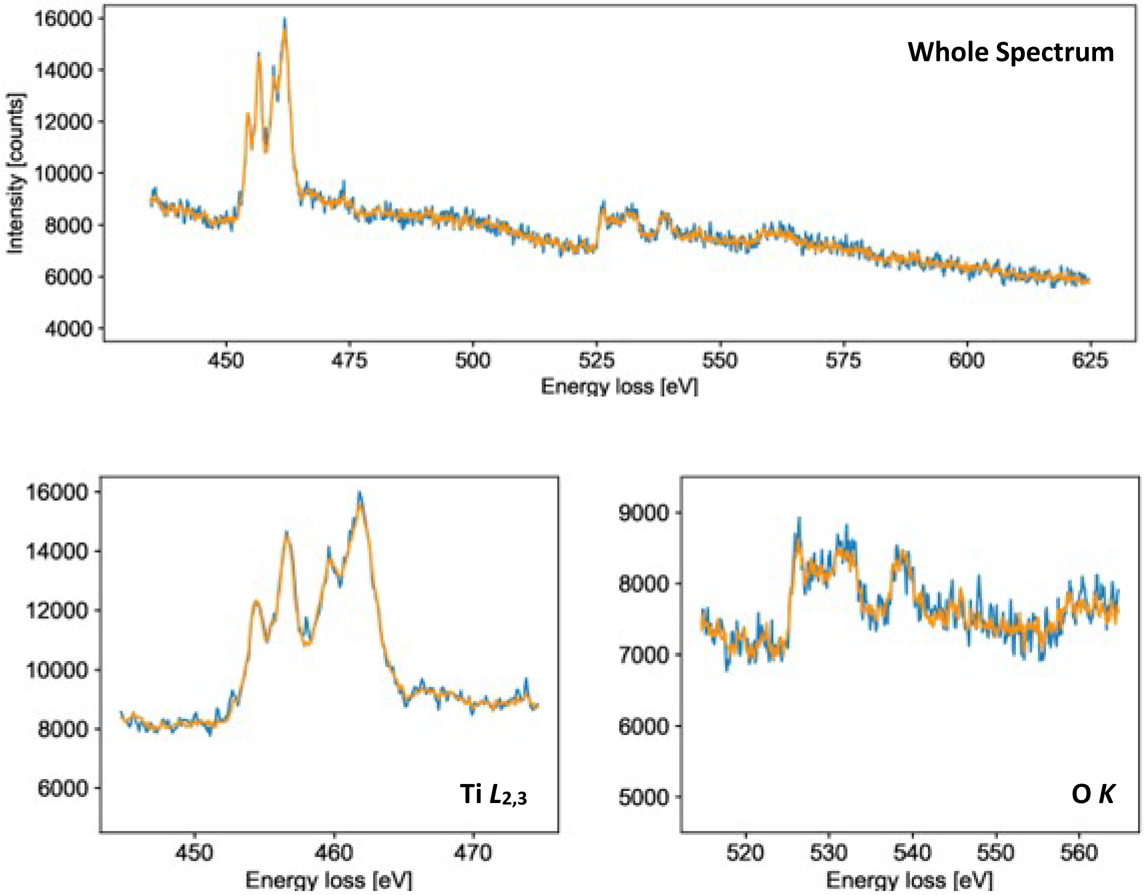


HAADF



Lewis et al. npj Comp. Mater., 8. 252. (2022).

Recurrent neural networks allow us to predict defect evolution to intelligently direct them



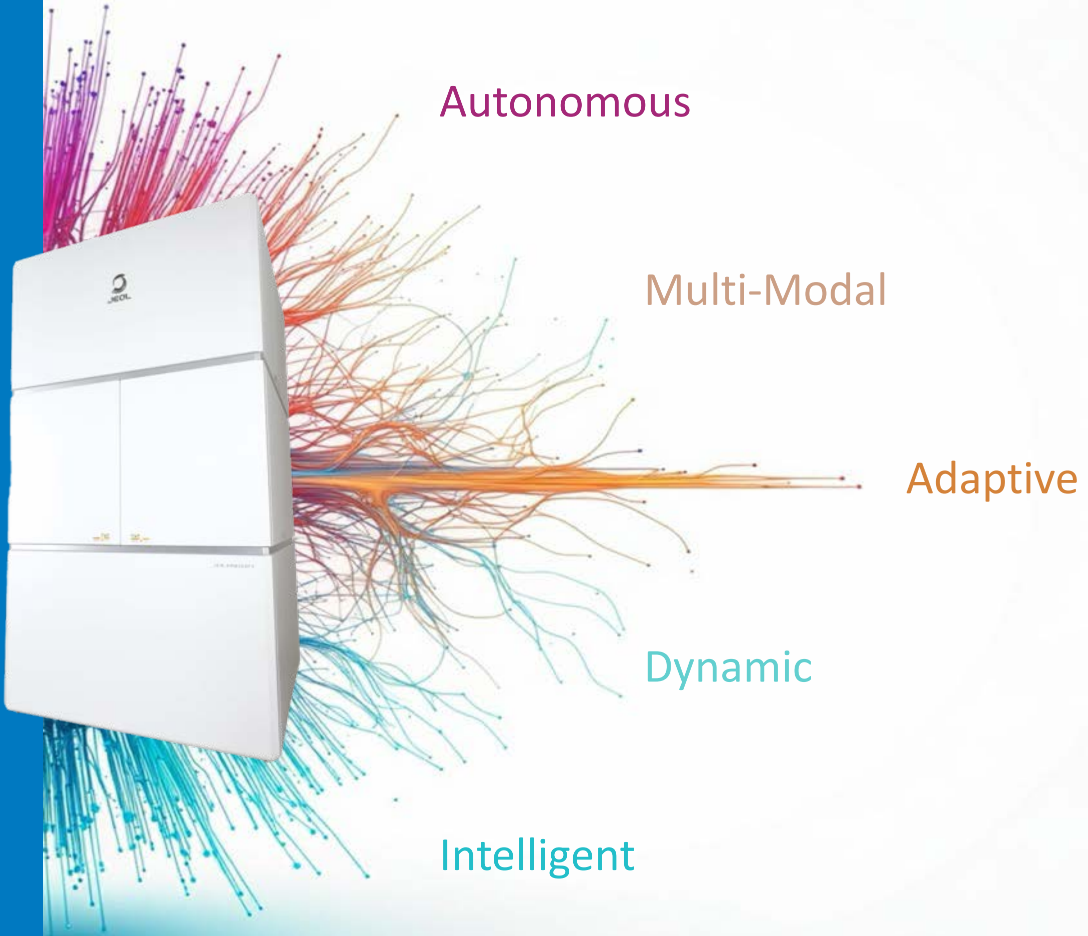
Lewis et al. npj Comp. Mater., 8. 252. (2022).

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

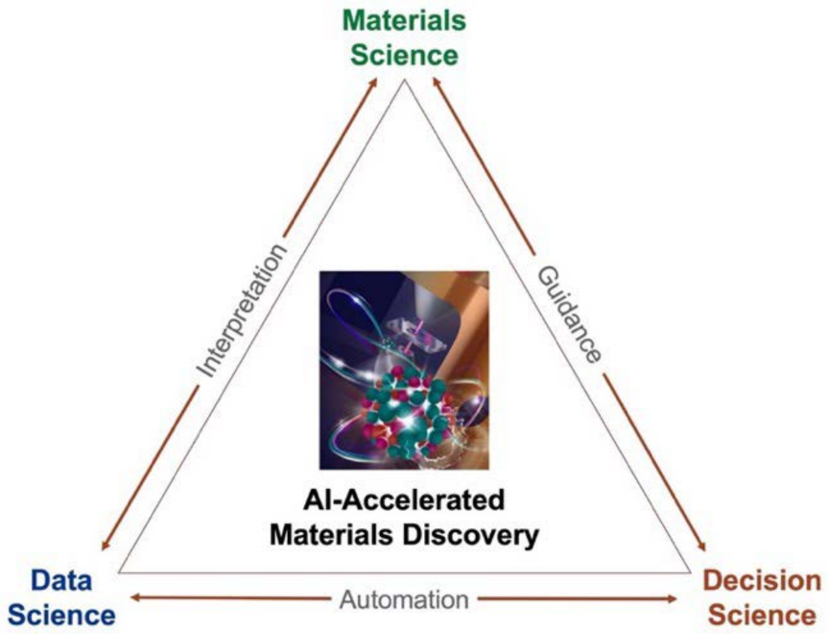


AM^3

The Autonomous Multi-Modal Microscope

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

For more information visit:
https://tinyurl.com/z8ryk4y3



NREL/PR-5K00-91779

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DOE Science Undergraduate Laboratory Internships (SULI)

- Internship Dates: Summer 2025
- Application Due: January 8, 2025
- 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 2025
- Apply: https://science.osti.gov/wdts/scgsr

SCAN ME

Contact me!

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UVa SULI Student Grace Guinan (Left) and NREL Postdoc Michelle Smeaton (Right)