

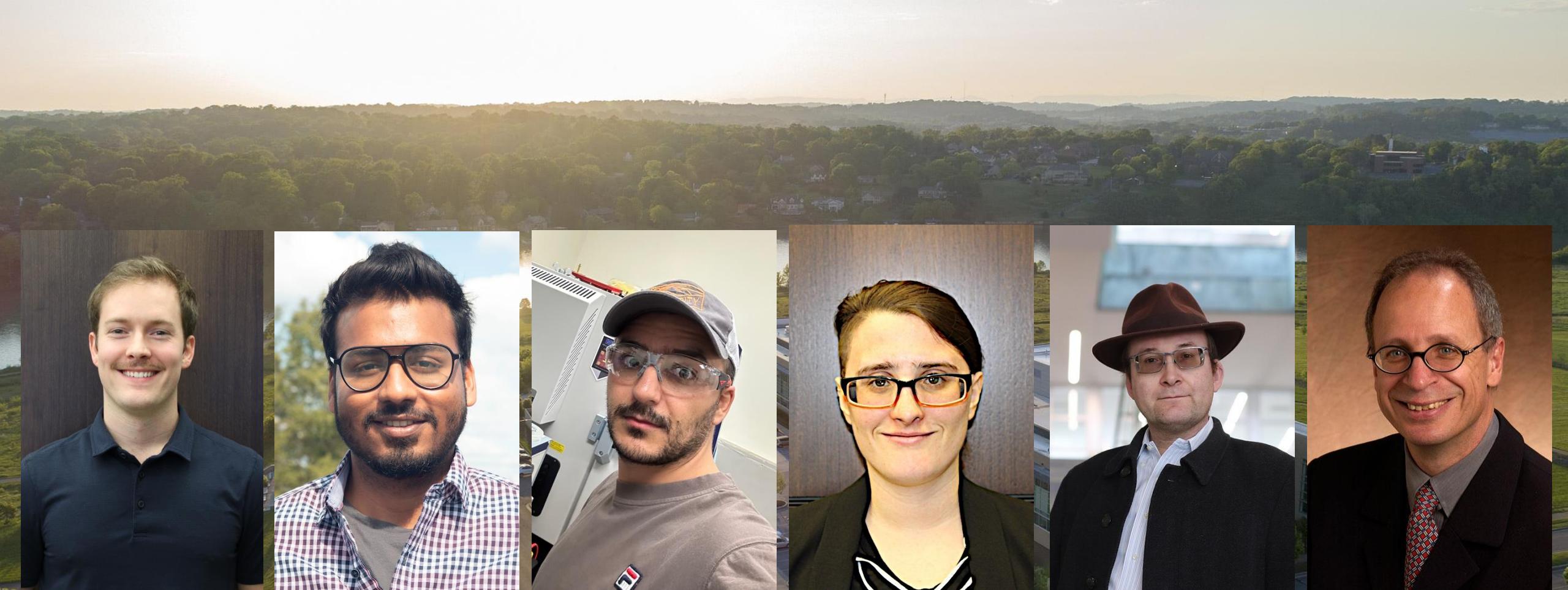
First ML Algorithms for Atomically Resolved Images

Austin Houston



THE UNIVERSITY OF
TENNESSEE
KNOXVILLE





Austin Houston

Utkarsh Pratiush

Kamyar Barakati

Elizabeth Heon

Sergei Kalinin

Gerd Duscher

Institute for Advanced
Materials and Manufacturing (IAMM)

Outline

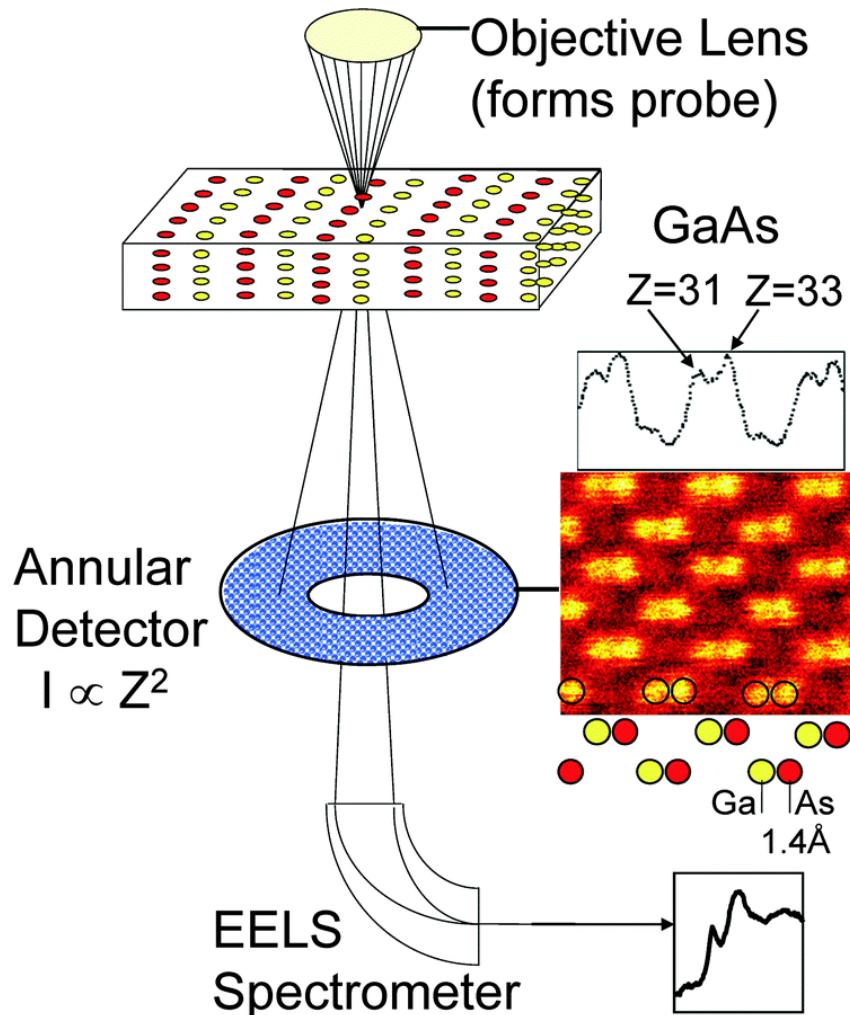
Atom positions are key

Dimensionality reduction methods

- First with atom positions
- Then, more generally

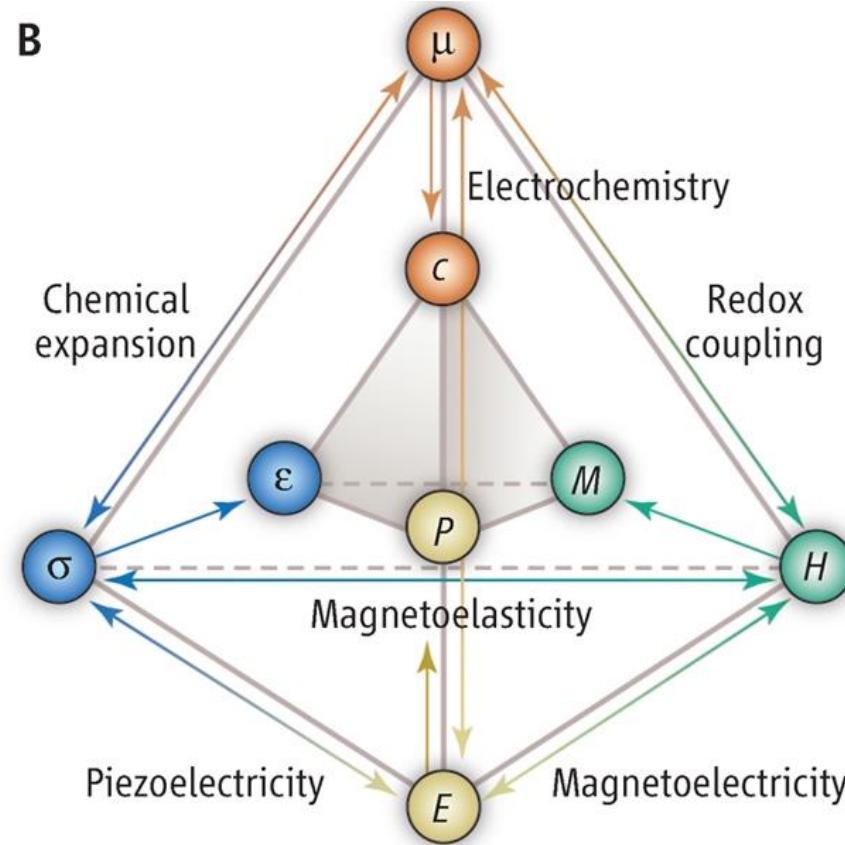
Hands-on notebook

HAADF STEM Imaging



Why do we want
to find atom
positions?

Local structure determines



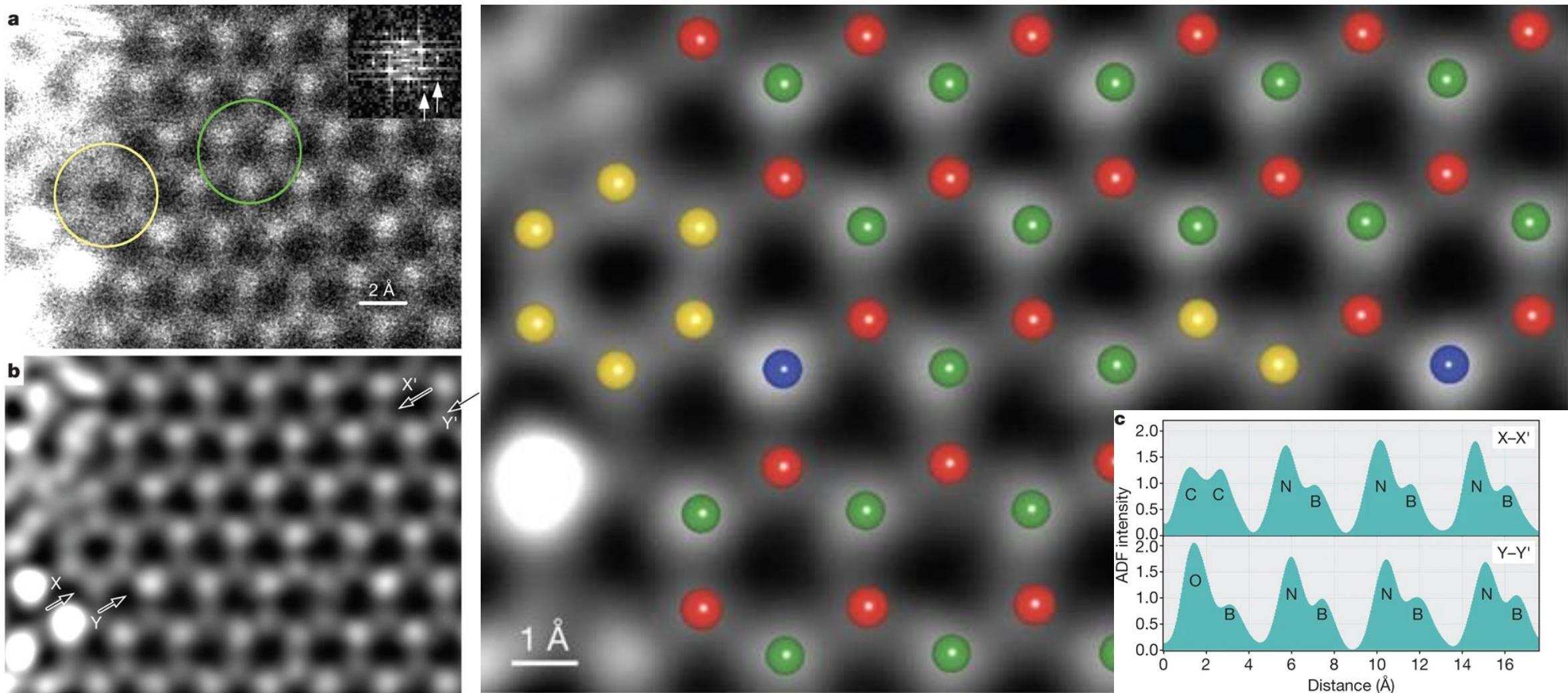
Kalinin and Spaldin, *Science* 2013

Natural Physics Descriptors

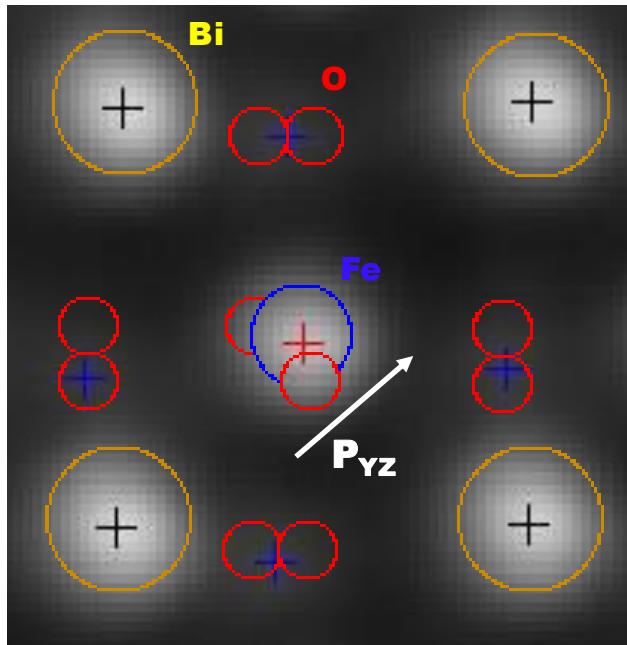
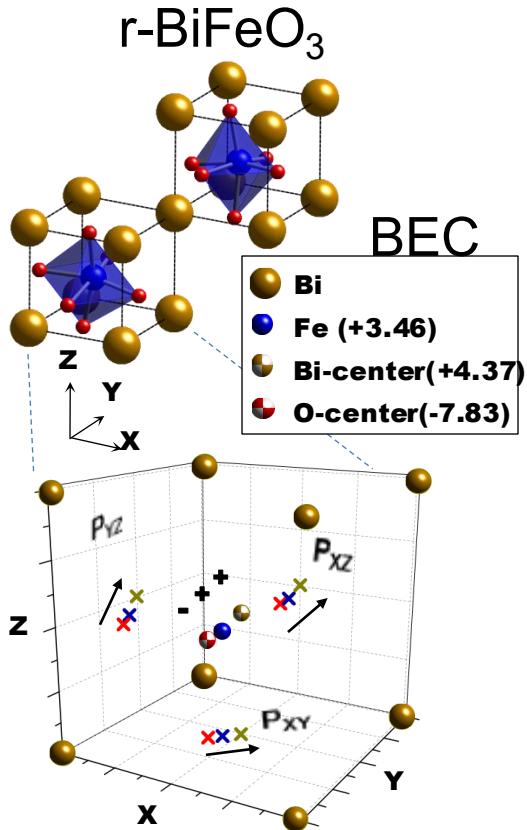
- Polarization
- Octahedra tilts
- Strains (physics and Vegard/chemical)

Caveat: STEM image is a projection. We have to treat image plane and beam direction differently

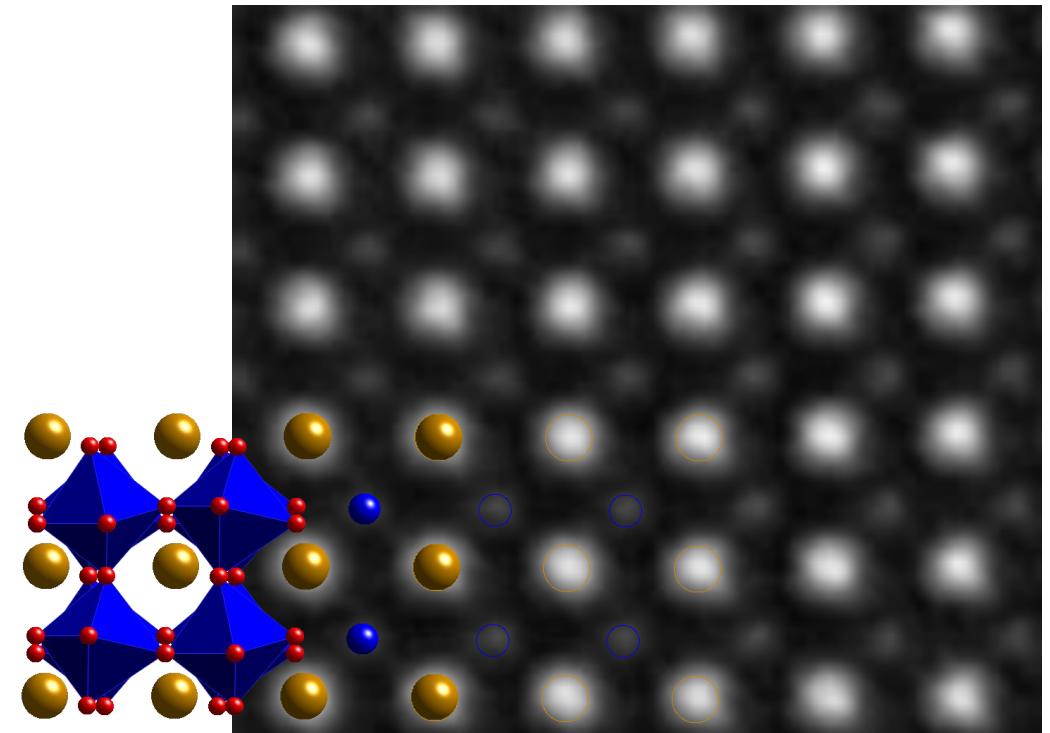
Chemistry



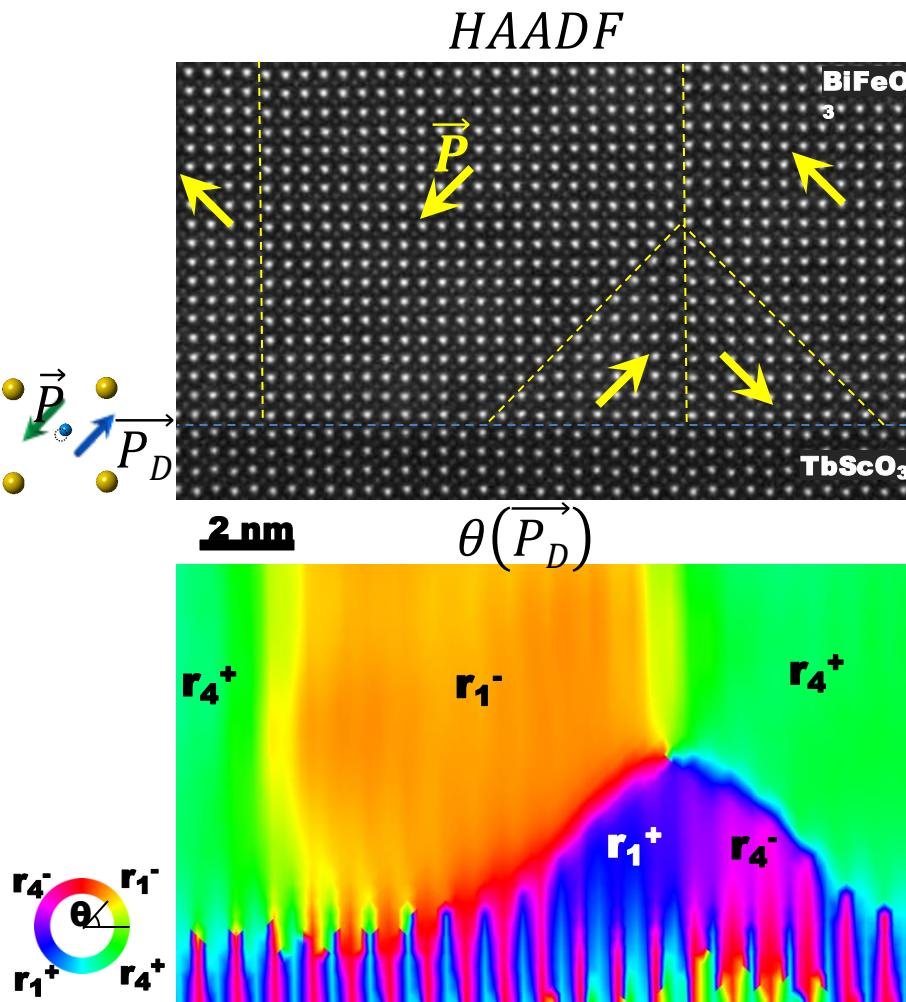
Polarization Imaging by STEM



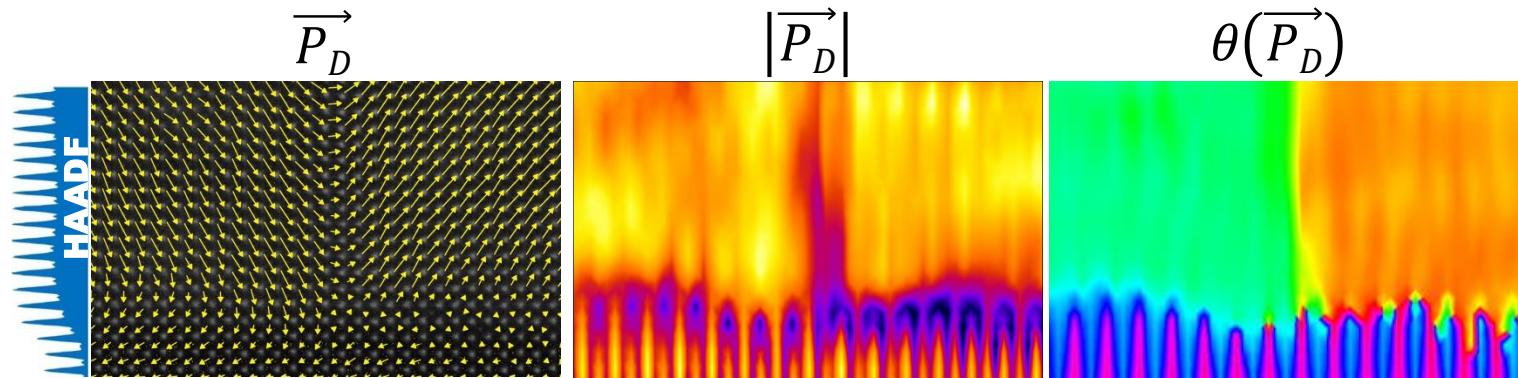
HAADF STEM



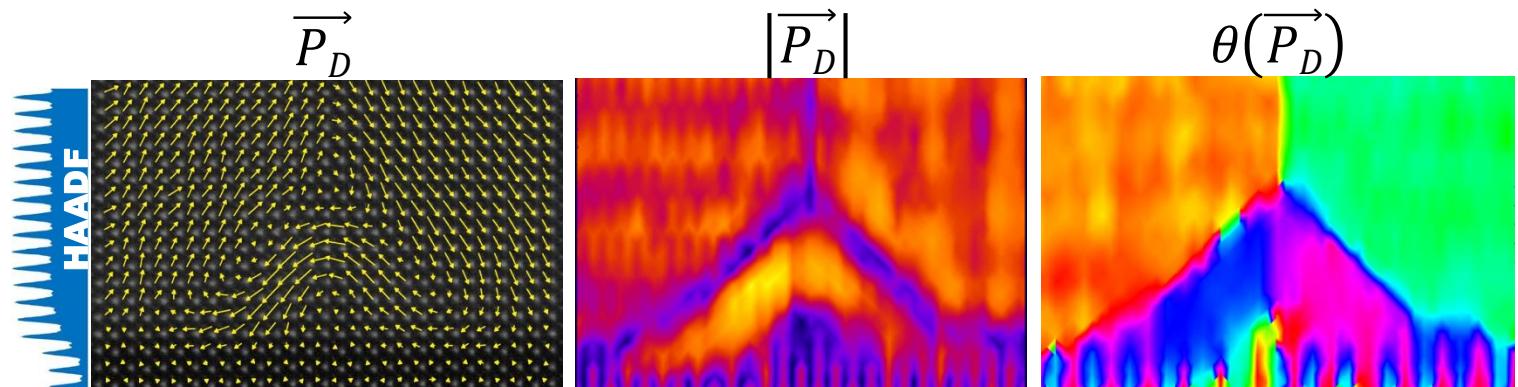
Polarization Imaging by STEM



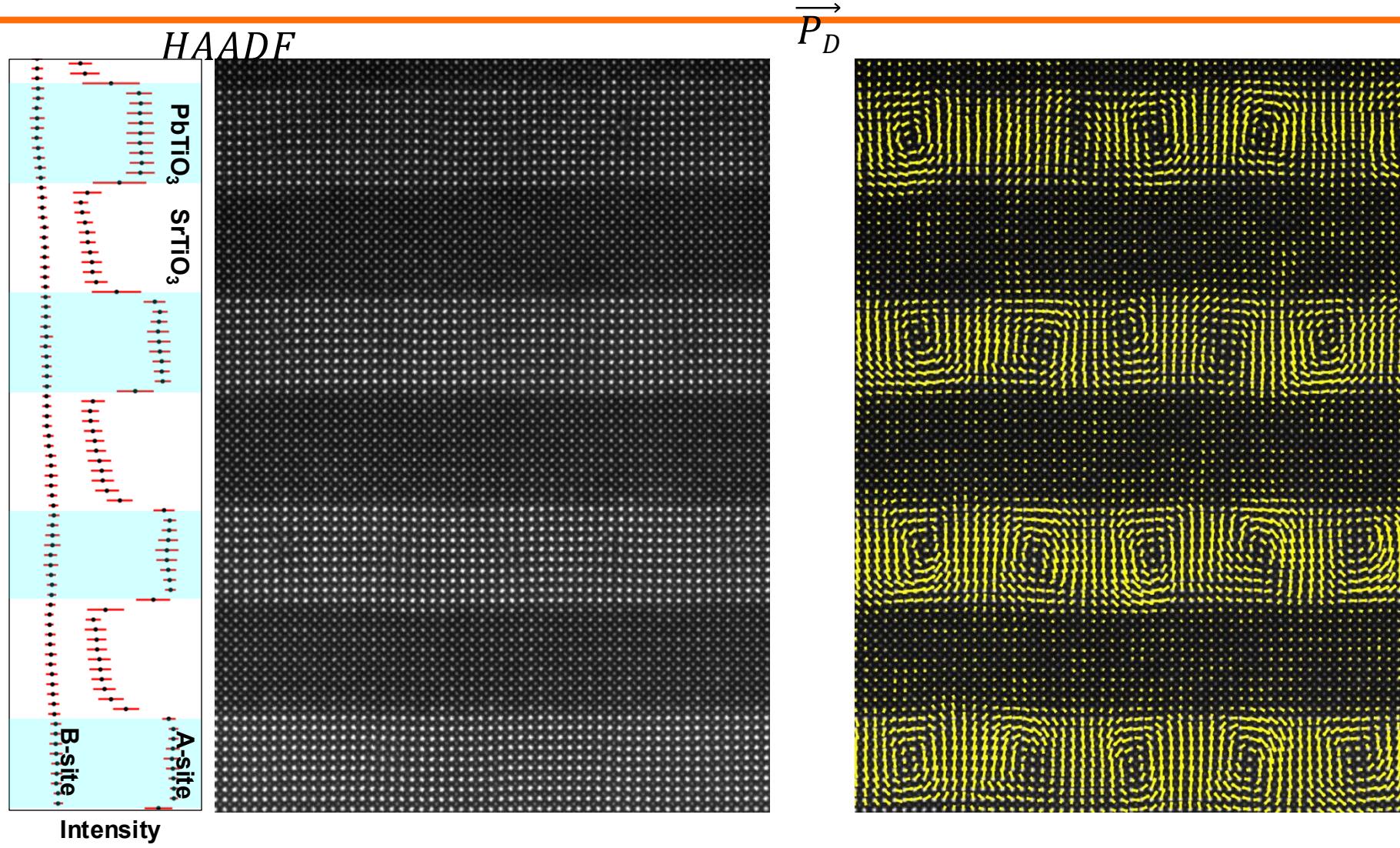
Direct Domain Wall Termination



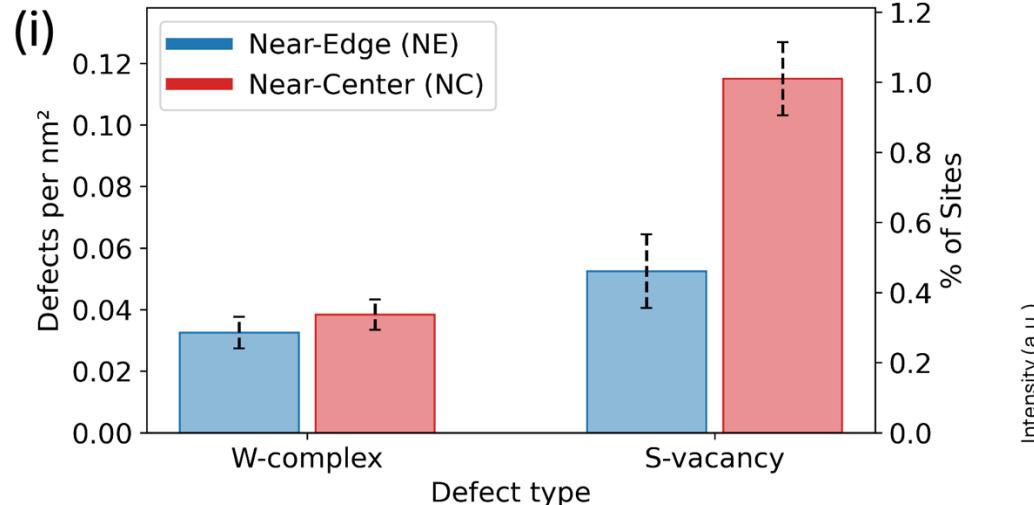
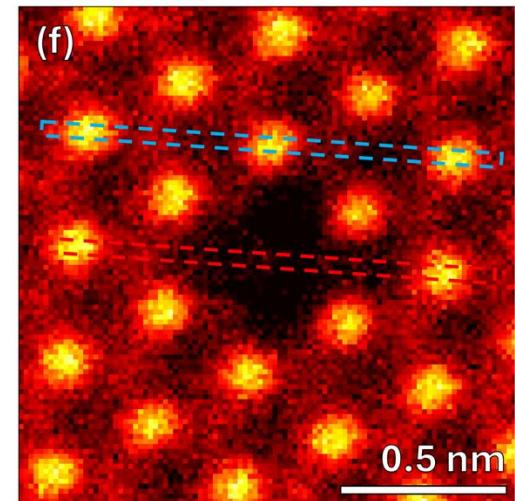
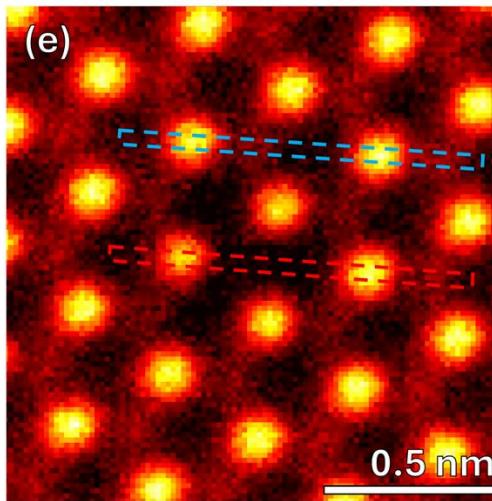
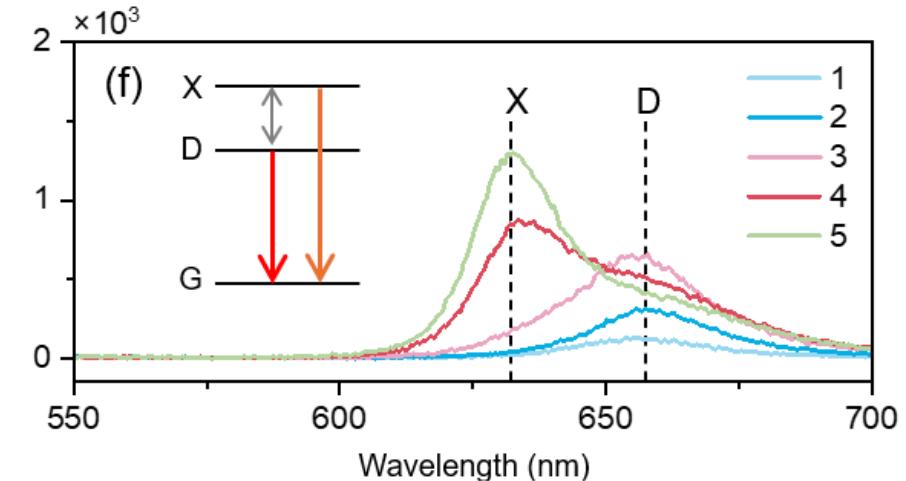
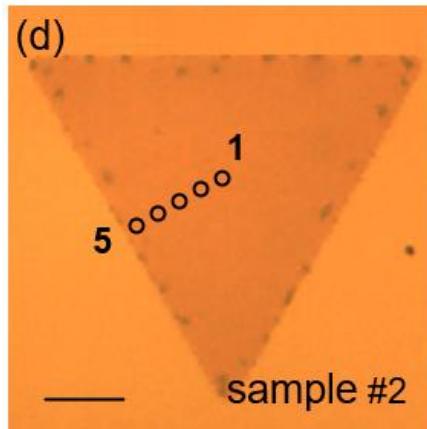
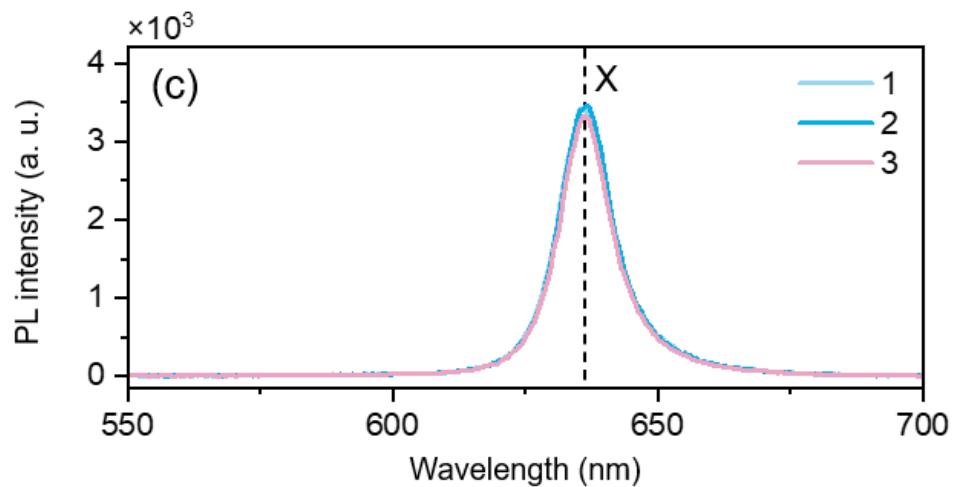
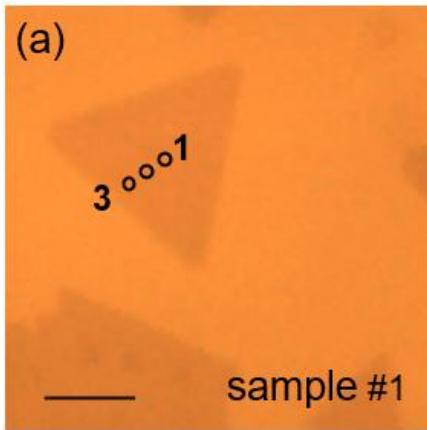
Flux-Closure at Domain Wall Termination



Polarization Imaging by STEM



Defect analysis



Atom Fabrication

nature reviews materials

Explore content ▾ About the journal ▾ Publish with us ▾

[nature](#) > [nature reviews materials](#) > [perspectives](#) > article

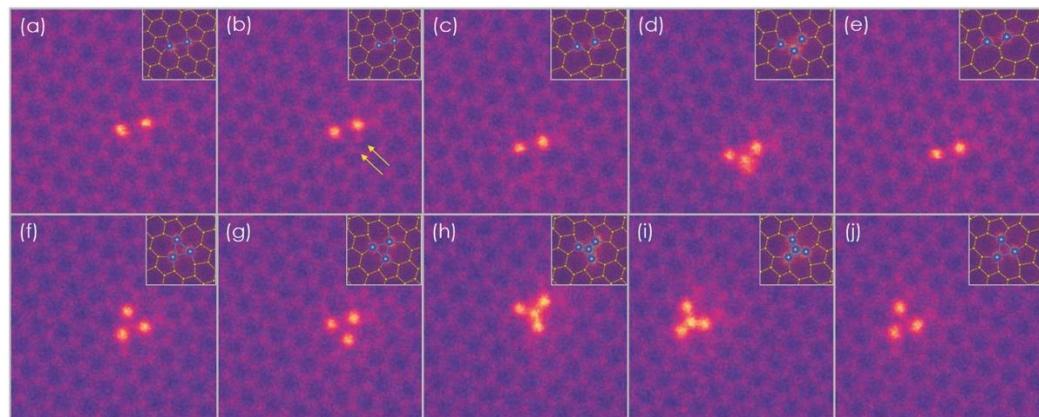
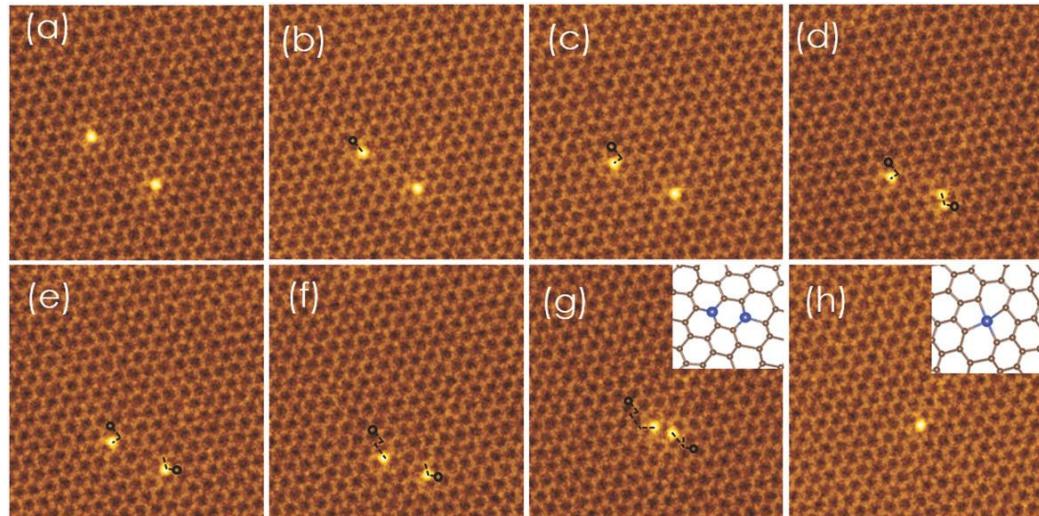
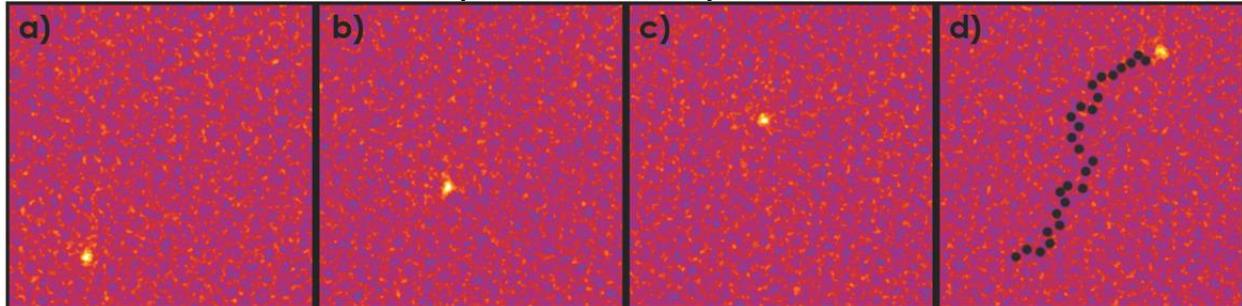
Perspective | Published: 07 June 2019

Atom-by-atom fabrication with electron beams

Ondrej Dyck , Maxim Ziatdinov, David B. Lingerfelt, Raymond R. Unocic, Bethany M. Hudak, Andrew R. Lupini, Stephen Jesse & Sergei V. Kalinin 

[Nature Reviews Materials](#) 4, 497–507 (2019) | [Cite this article](#)

Disclaimer: beam was positioned by hand



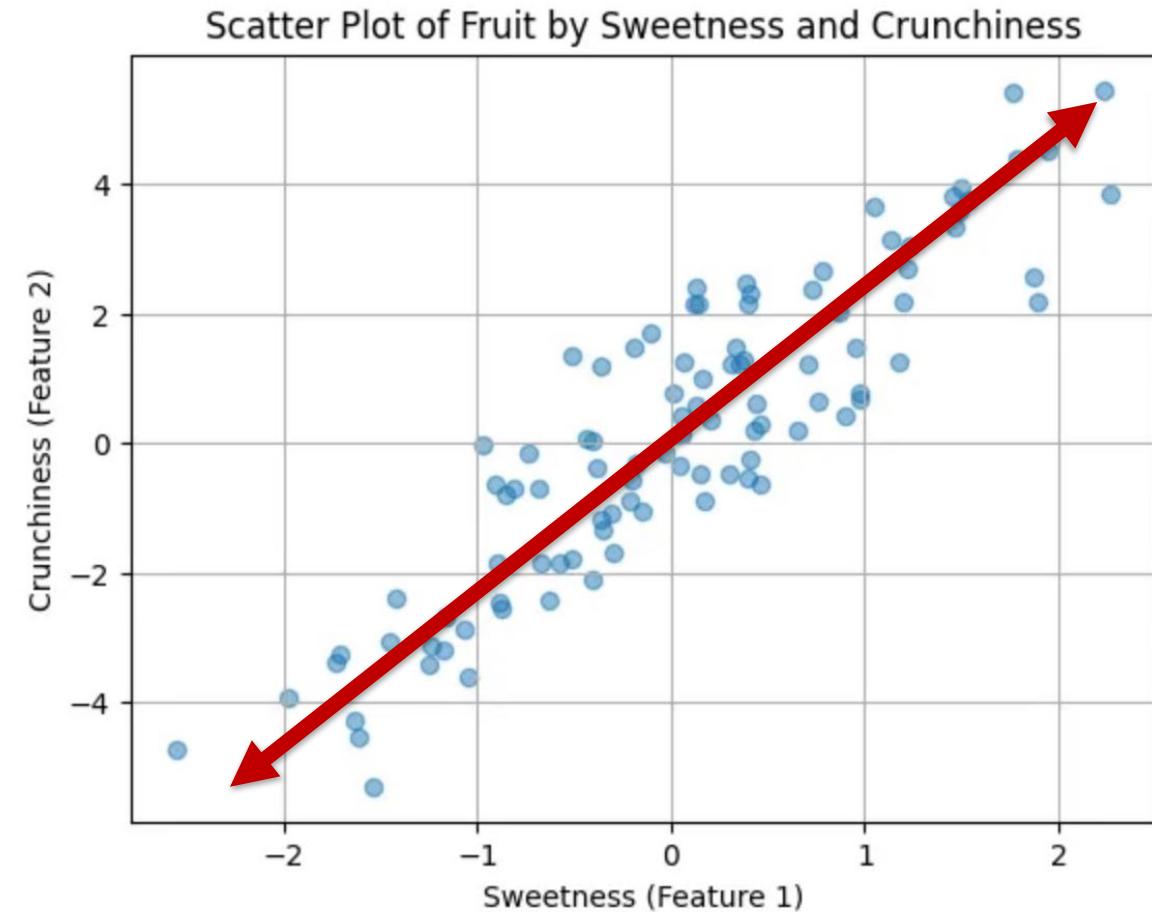
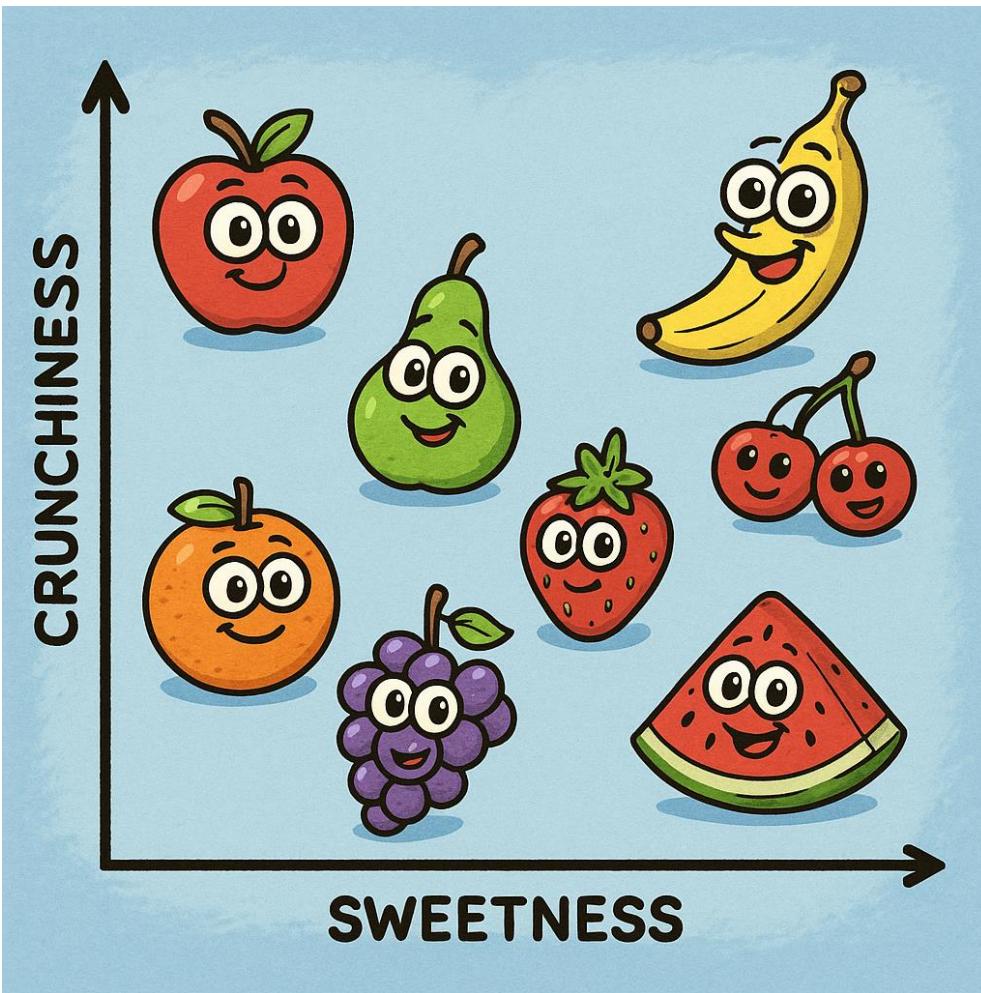
First Approaches

MACHINE LEARNING

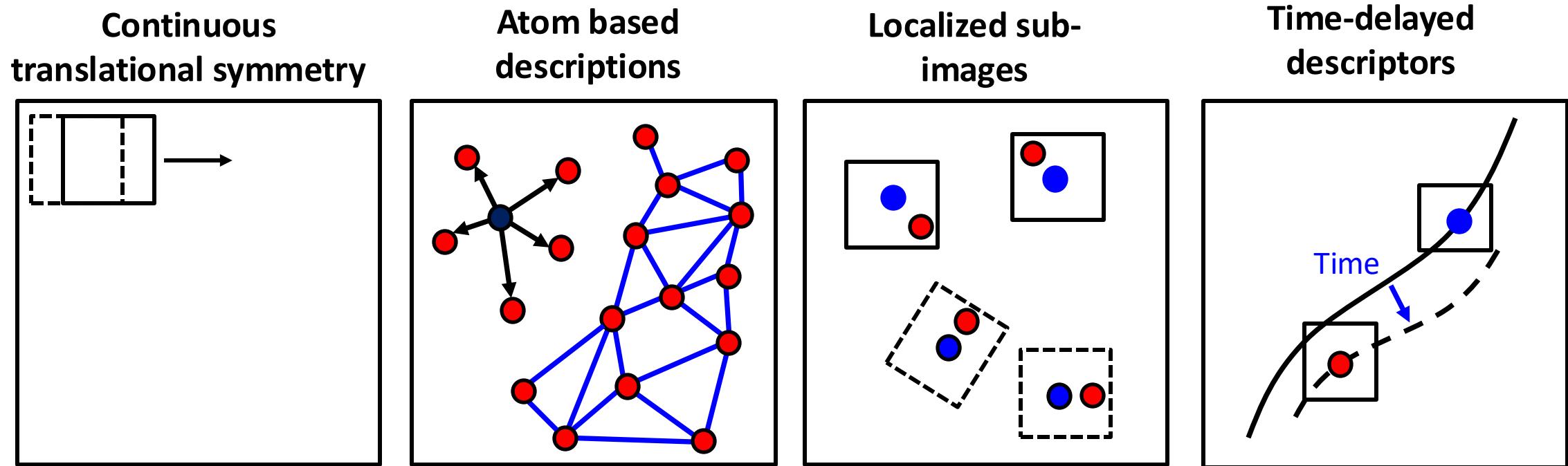
Principal Component Analysis

- Reveals internal structure of the data that best explains variance in the data set
 - PCA transforms the data such that the greatest variance by any projection lies on the first coordinate
-
1. **Center the data** by subtracting the mean of each feature
 2. **Compute the covariance matrix** of the centered data, which captures how features vary together.
 3. **Calculate the eigenvectors and eigenvalues** of this covariance matrix.
 4. The **first principal component** is the eigenvector with the largest eigenvalue — i.e., the direction of maximum variance.
 5. Subsequent components are the eigenvectors with the next largest eigenvalues, and they are **all orthogonal** (uncorrelated) to each other.

Principal Component Analysis



Constructing the descriptors

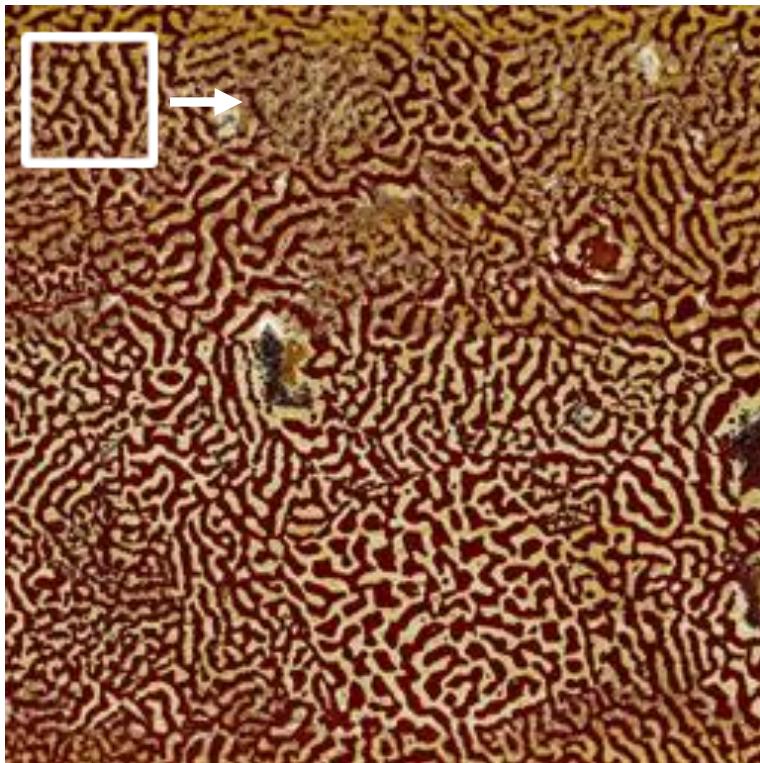


The choice of the descriptor:

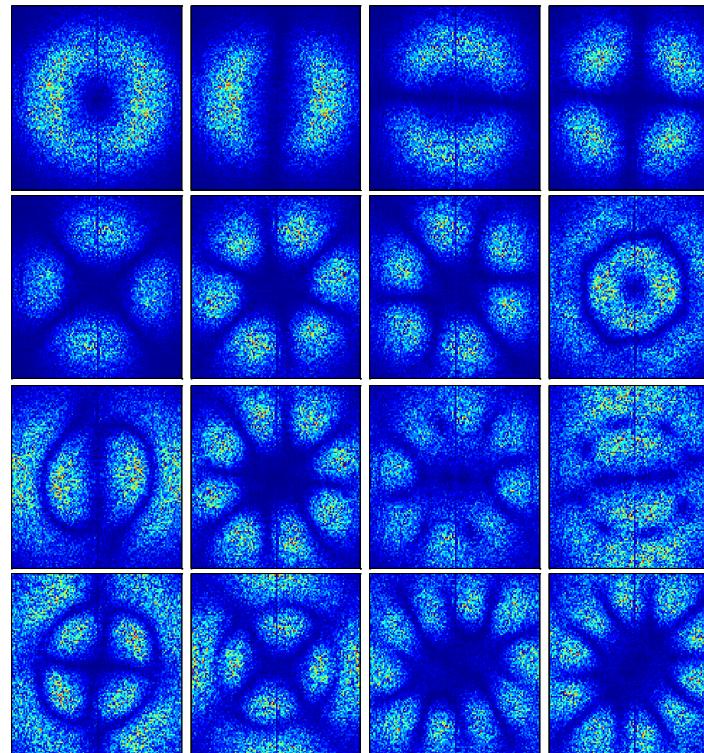
- Defines physical inferential biases and allows to introduce prior knowledge
- Determines the physical meaning of the analysis
- Establishes the analysis pipeline

Sliding PCA-FFT

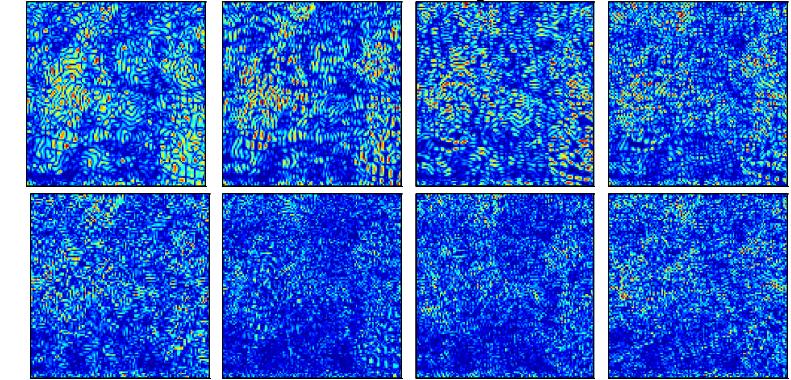
Can we use PCA of FFT in sliding windows to find periodicity?



First 16 eigenvectors



First 8 maps



The last 8 components are randomly distributed and small

Sliding FFT:

We always have a problem of window size:

- o too large – loose spatial resolution,
- o too small – FFT behaves poorly due to edge effects

Interpretation of FFT data is complicated (too much data if fit each peak, unclear meaning of the unmixing components)

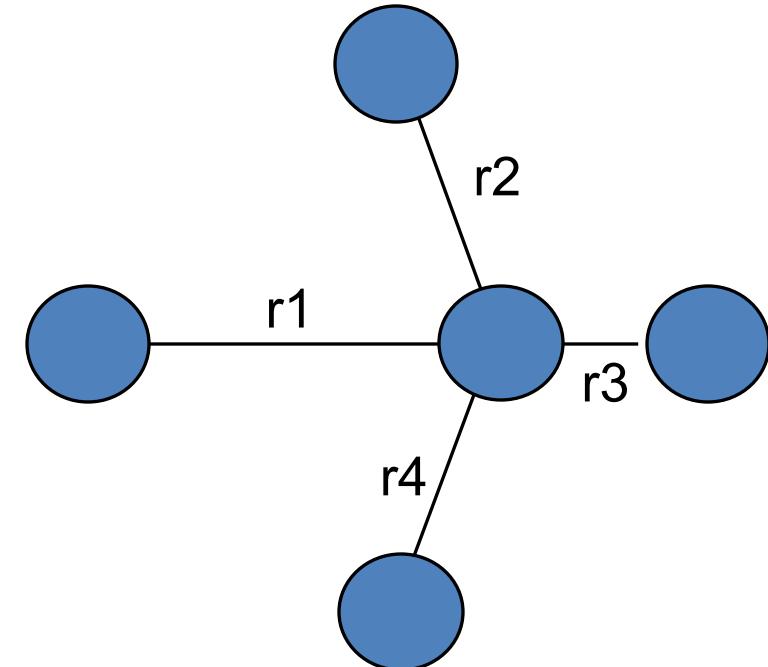
Natural descriptor for atomically resolved images – atomic coordinates!

Nearest neighbor descriptors

For each atom, define nearest neighbors and generate array of the corresponding radius-vectors of the form

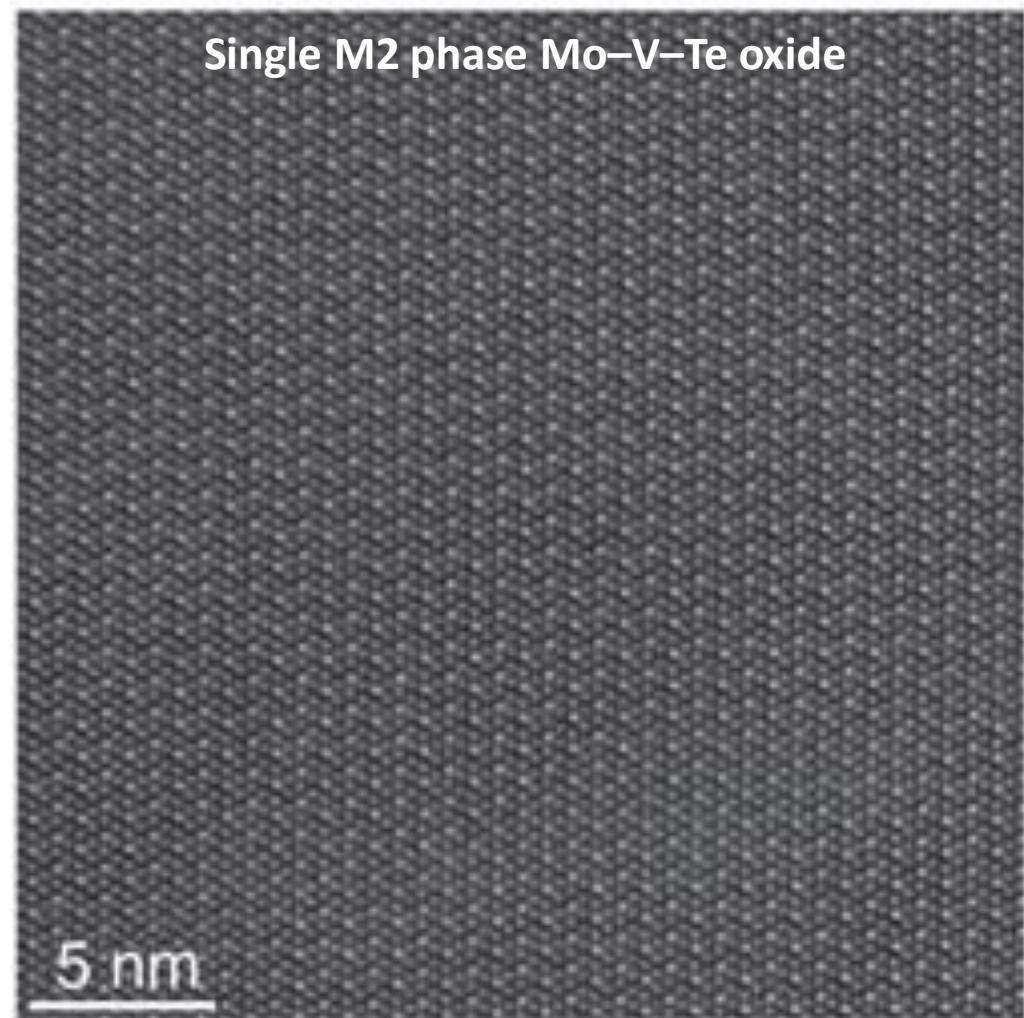
$$NA_{ij} = (rx_1, ry_1, rx_2, ry_2, rx_3, ry_3, rx_4, ry_4)_{ij}$$

Indexes 1,2,3,4 are chosen in the same sense for all atoms



Local crystallography

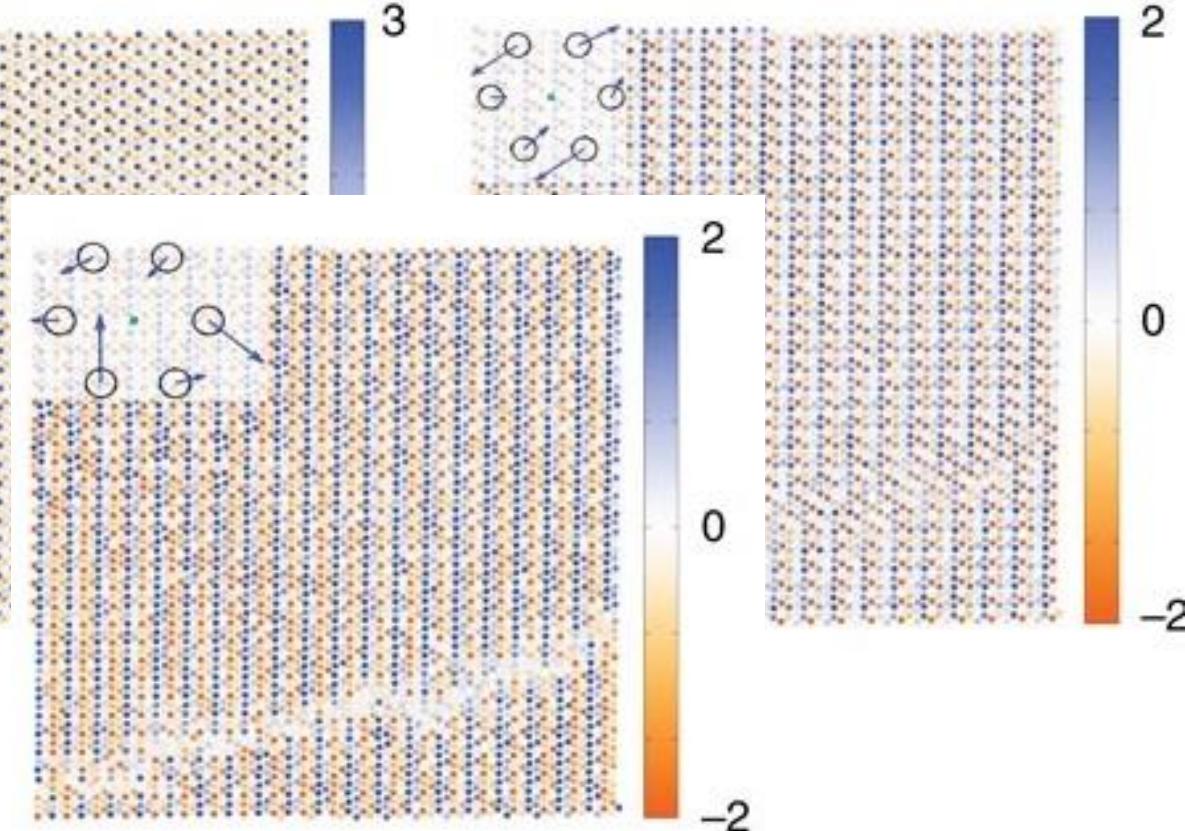
Single M2 phase Mo–V–Te oxide



Polar shift

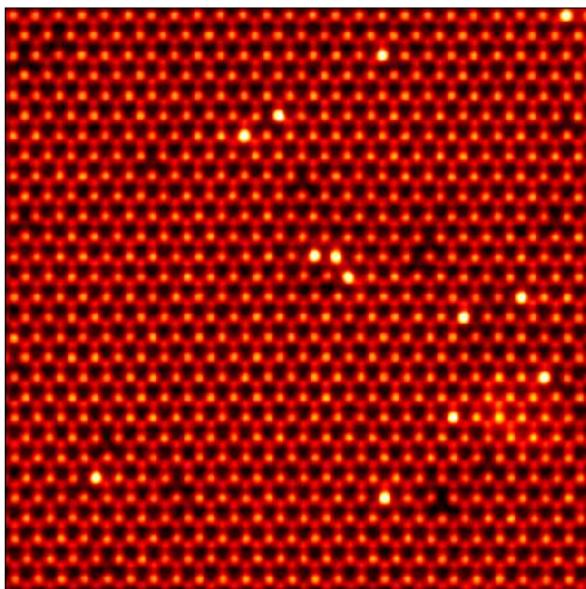


Shear mode

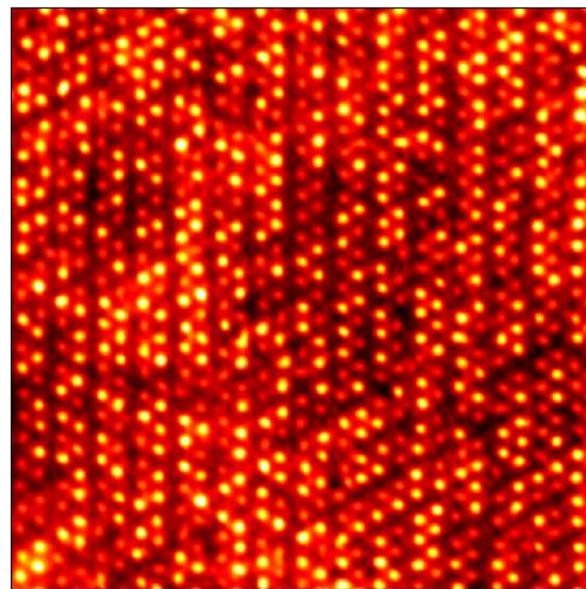


MoS₂-ReS₂

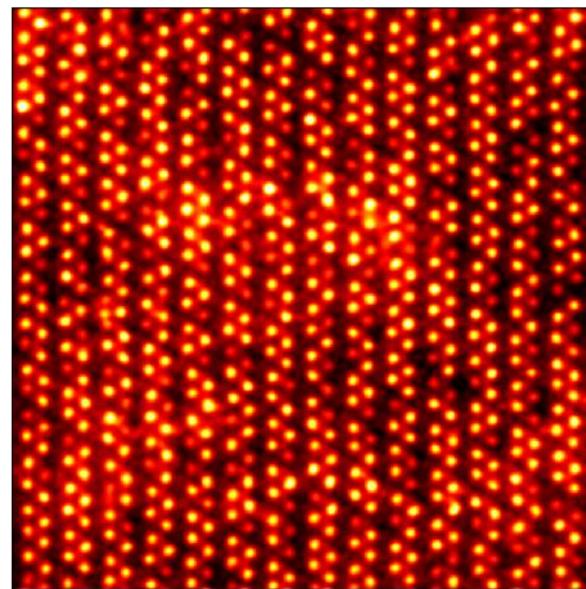
5% ReS₂



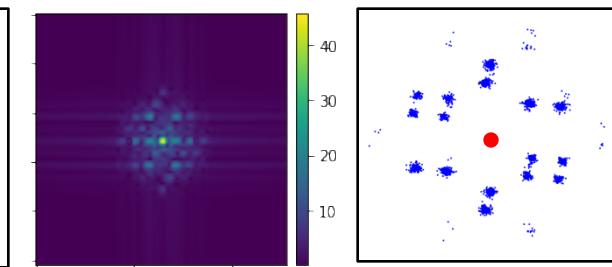
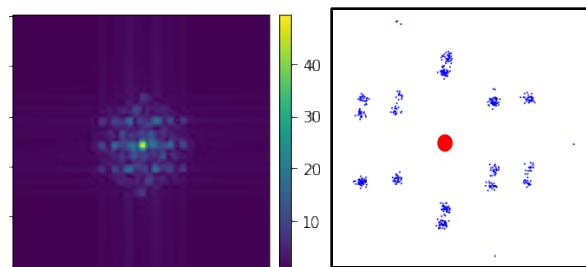
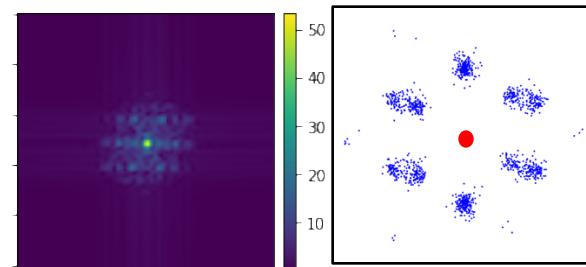
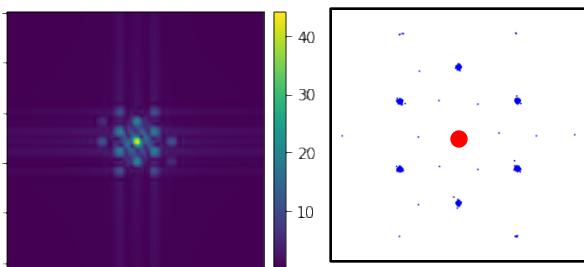
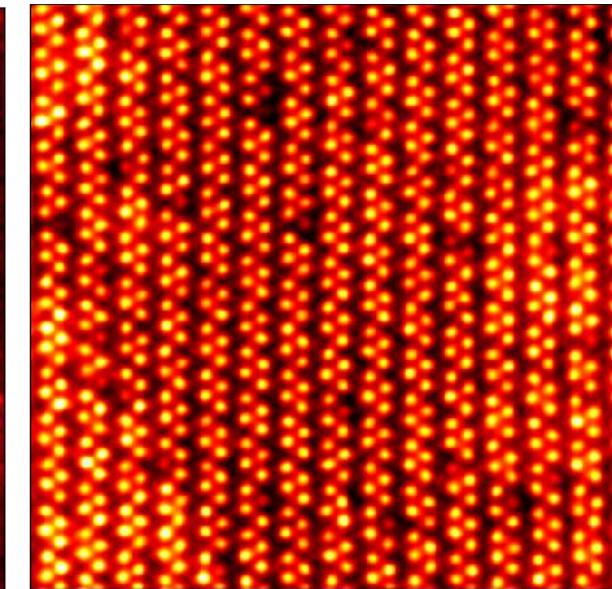
55% ReS₂



78% ReS₂



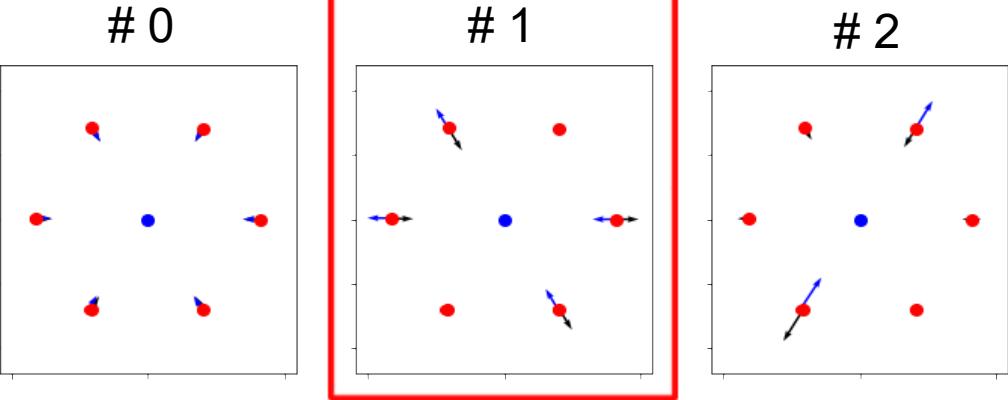
95% ReS₂



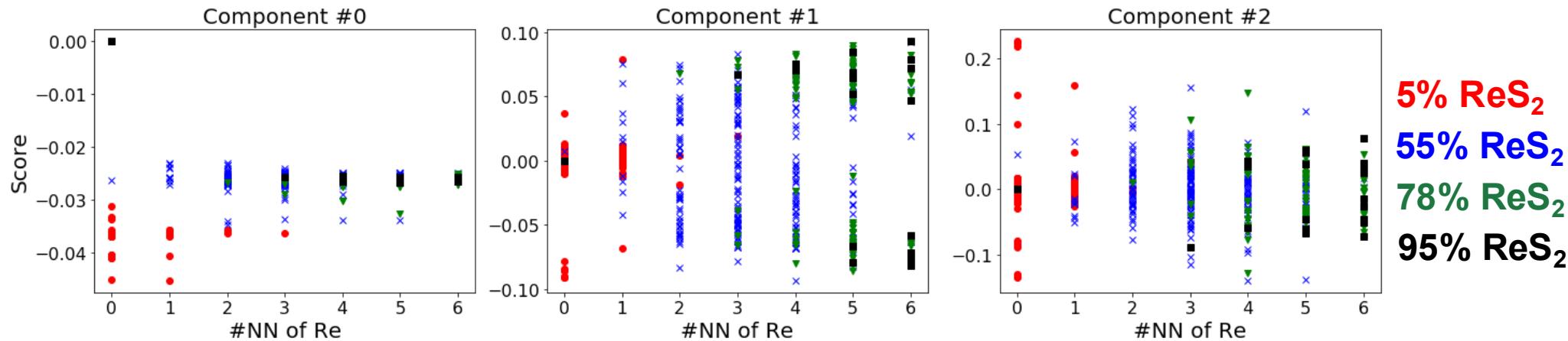
Data by Shize Yang and Matt Chisholm

Describing the phase transition

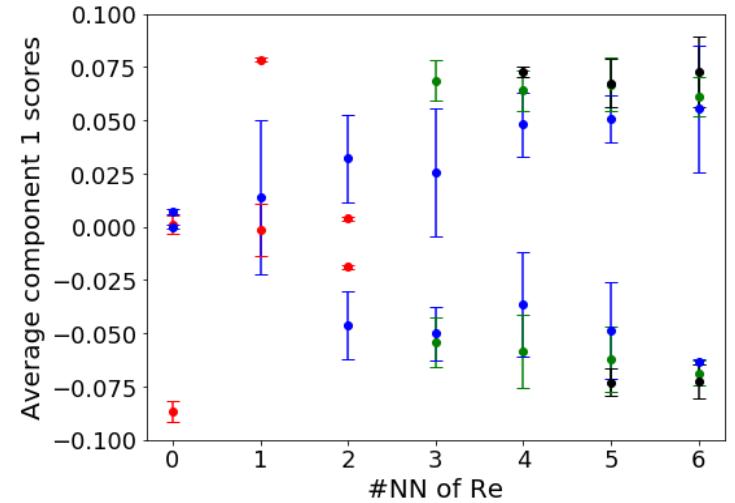
Three dominant distortion modes



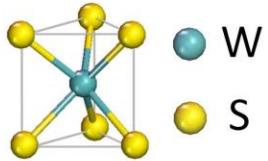
Mode distributions vs. global and local composition



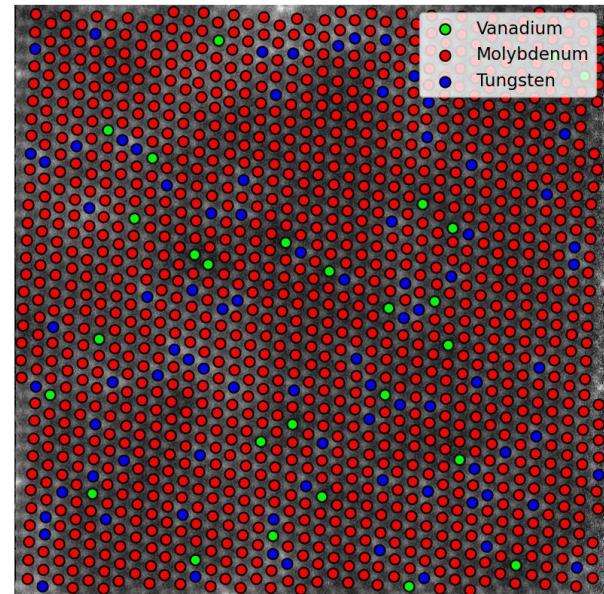
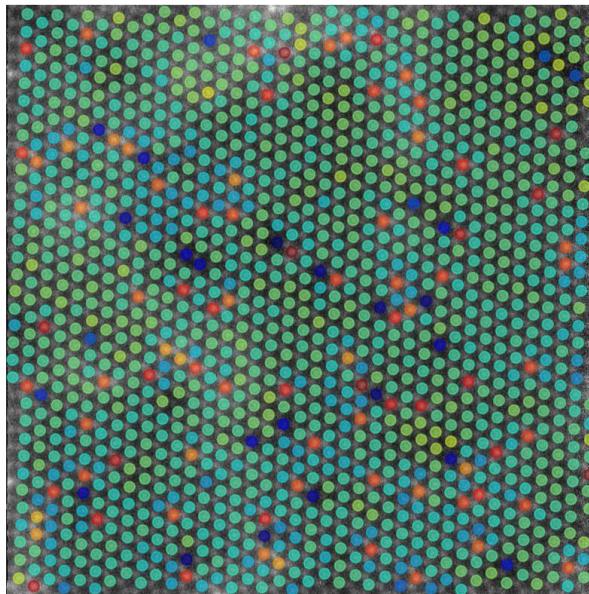
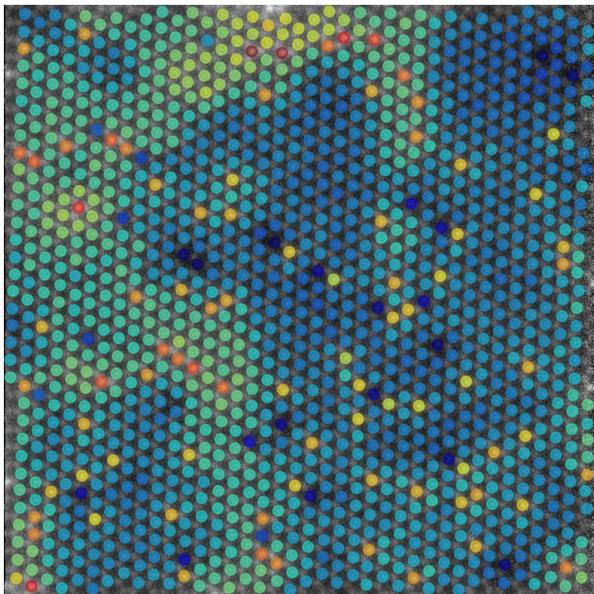
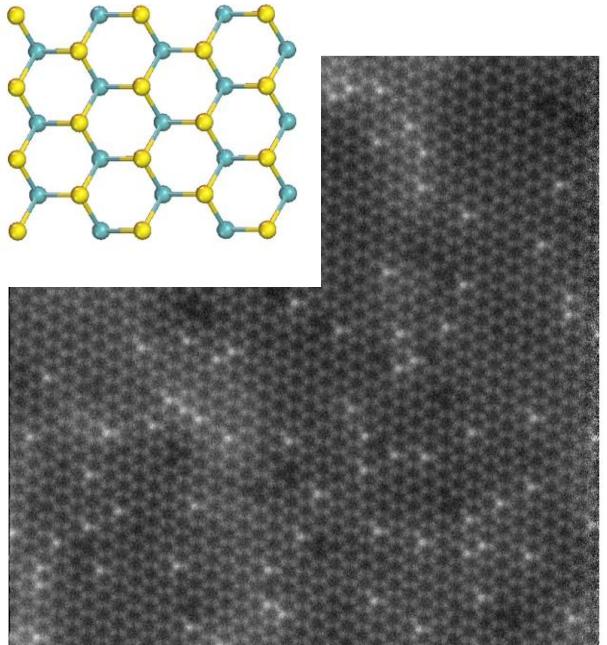
Local symmetry breaking!



Hands-on notebook



W
S



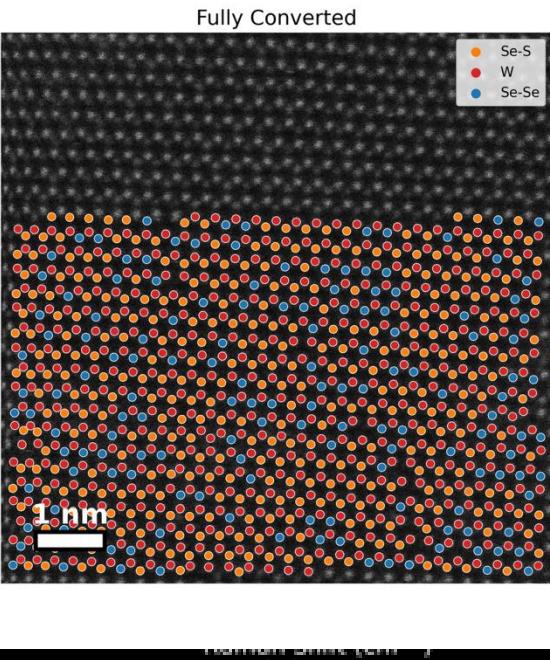
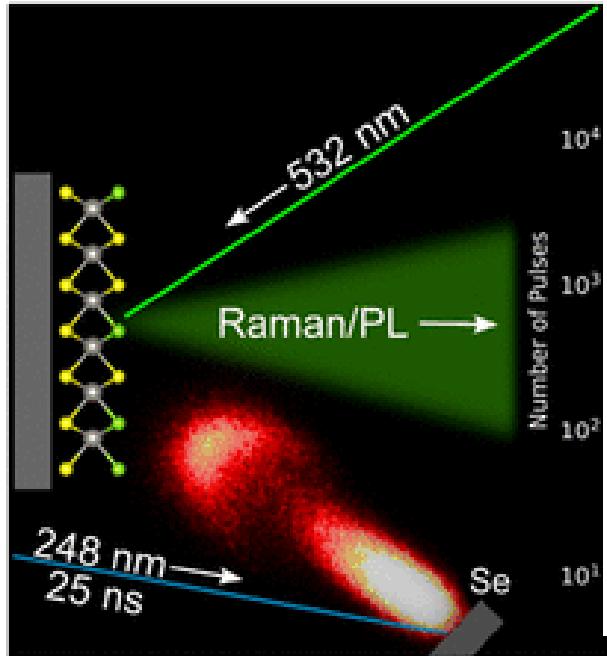


Thank you!

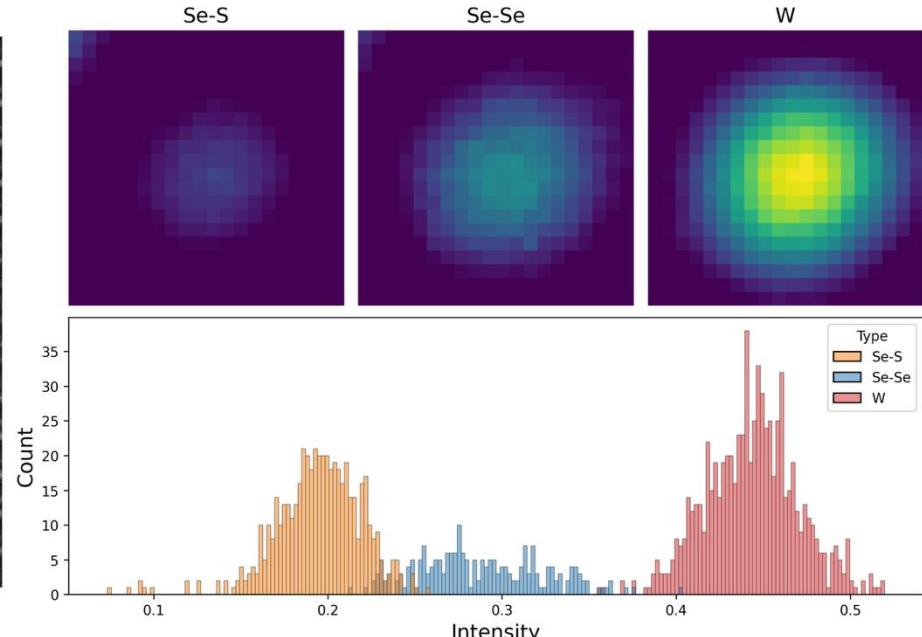


THE UNIVERSITY OF
TENNESSEE
KNOXVILLE

Outline



Tile-based Clustering



Cite Share Jump to Expand

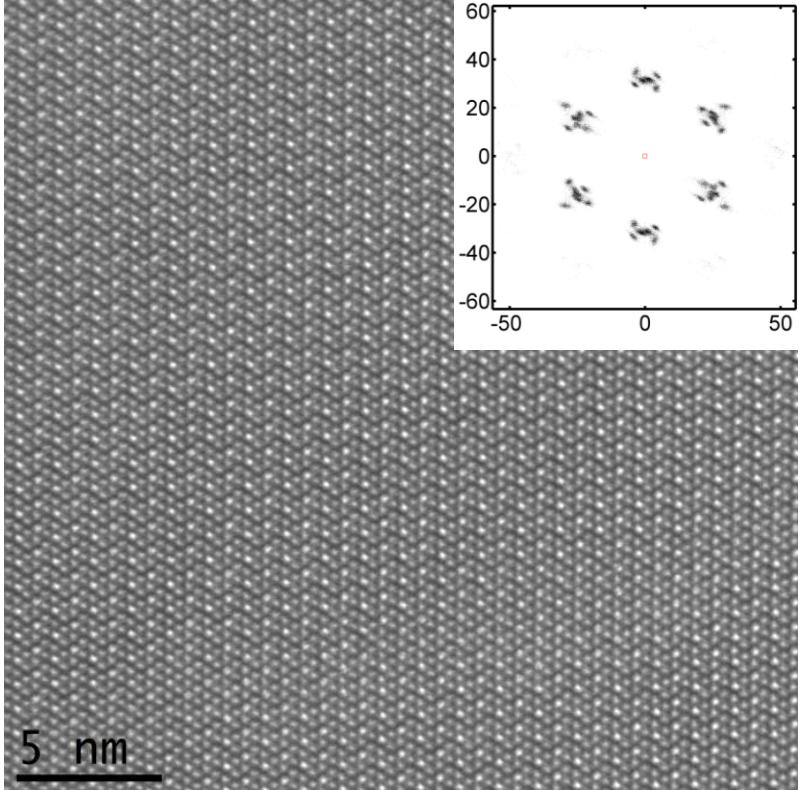
ARTICLE | January 17, 2023

Real-Time Diagnostics of 2D Crystal Transformations by Pulsed Laser Deposition: Controlled Synthesis of Janus WSSe Monolayers and Alloys

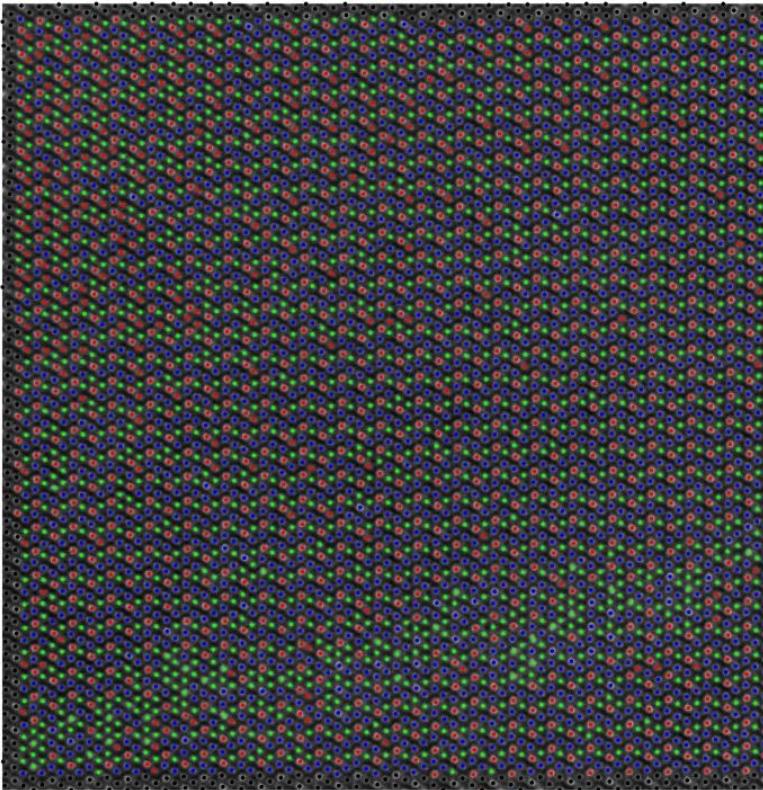
Sumner B. Harris, Yu-Chuan Lin, Alexander A. Puretzky, Liangbo Liang, Ondrej Dyck, Tom Berlijn, Gyula Eres, Christopher M. Rouleau, Kai Xiao, and David B. Geohegan*

Local crystallography

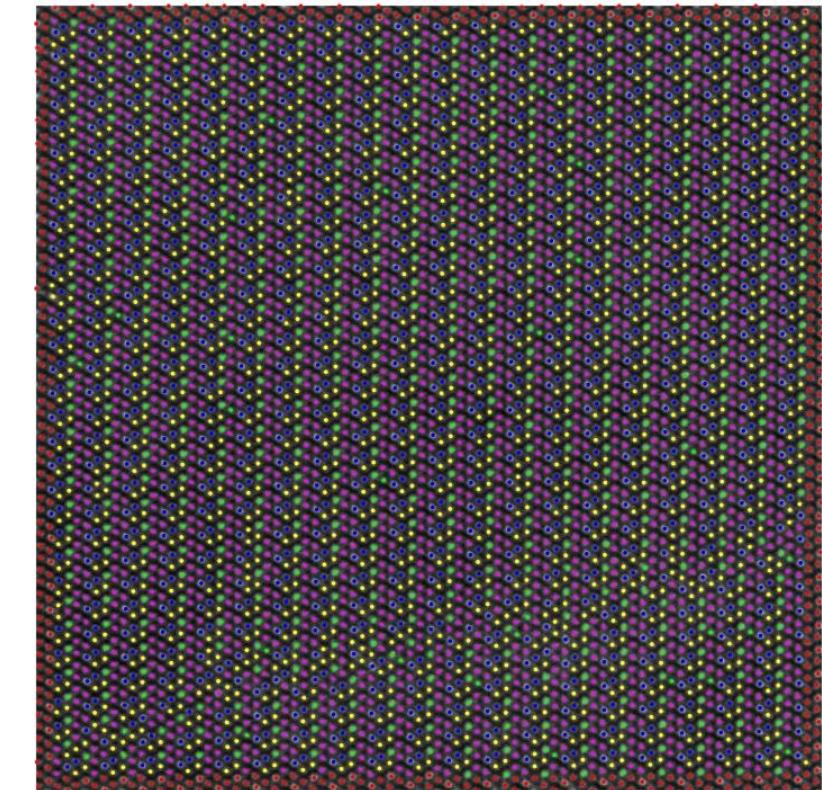
Image



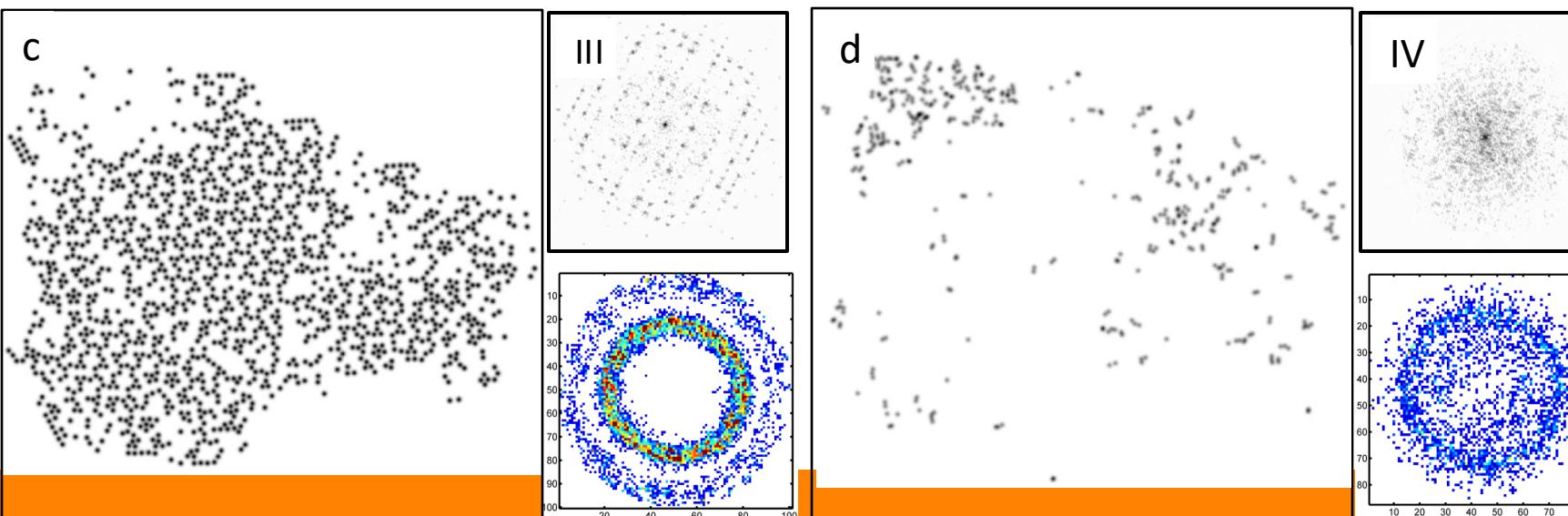
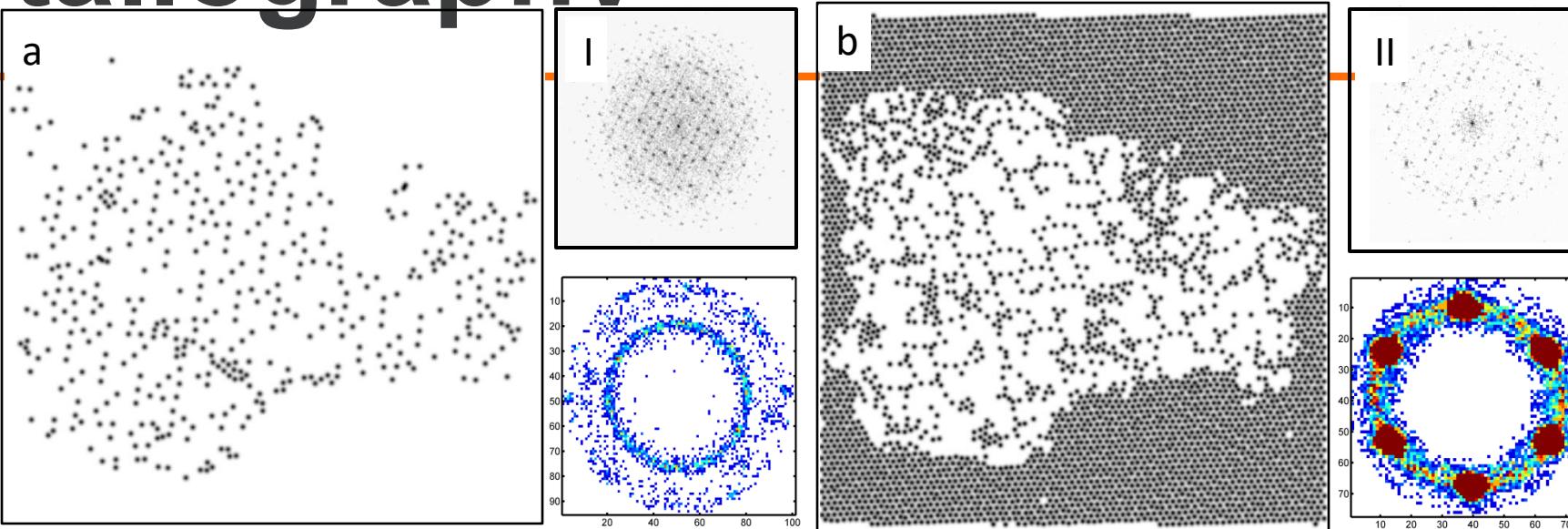
K-means full radius vector



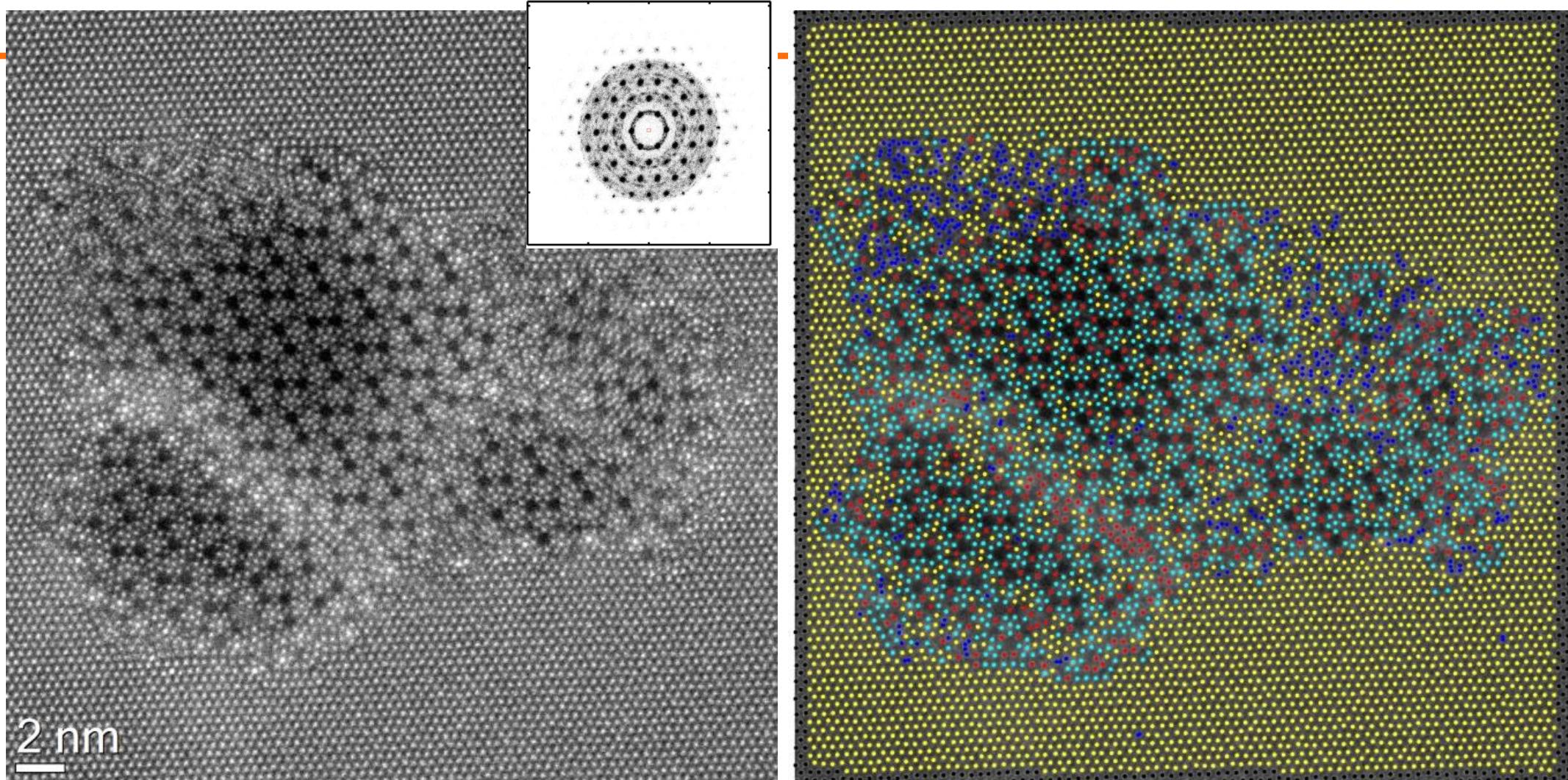
K-means angles



Local crystallography



Local crystallography: k-means



A. BELIANINOV, Q. HE, M. KRAVCHENKO, S. JESSE, A. BORISEVICH, and S.V. KALININ, *Identification of phases, symmetries, and defects through local crystallography*, Nat. Comm. **6**, 7801 (2015).