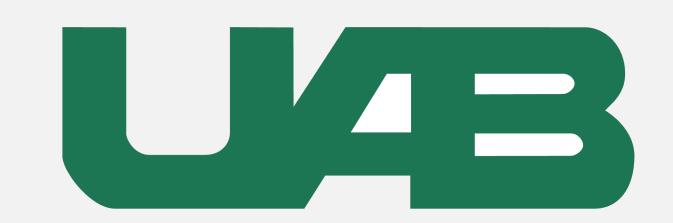
ANALYZING NANOSCALE HYPERSPECTRAL DATASETS OF HYBRID PEROVSKITES WITH MACHINE LEARNING



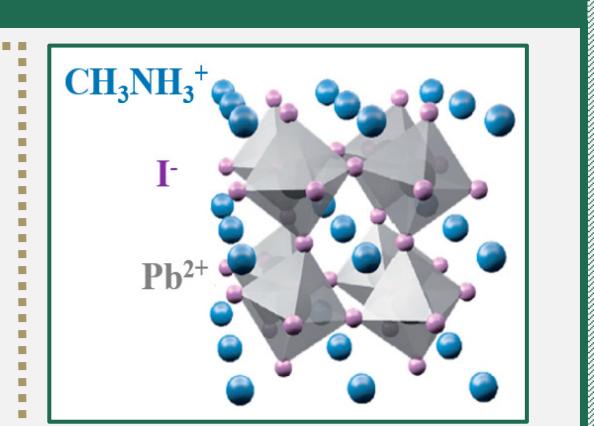
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MOTIVATION

BACKGROUND

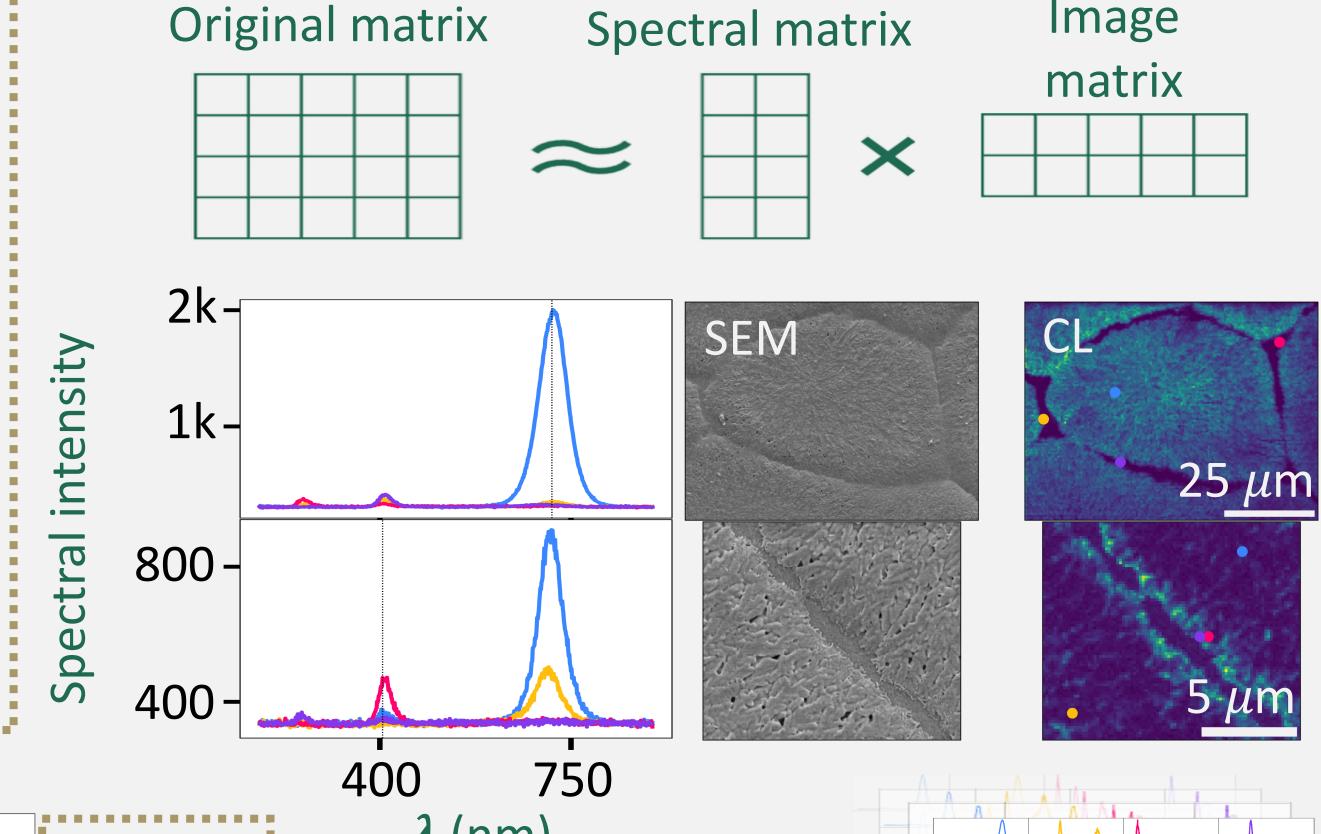
- Hybrid perovskites (HP's) have recently generated unprecedented growth in opto-electronic technologies.
- Used in photovoltaics (solar cells), light-emitting diodes, Machine learning is neuromorphic computing...
- Deeper understanding of phase stabilization is critically needed



increasingly being used to understand complex data in novel ways beyond numan perception.

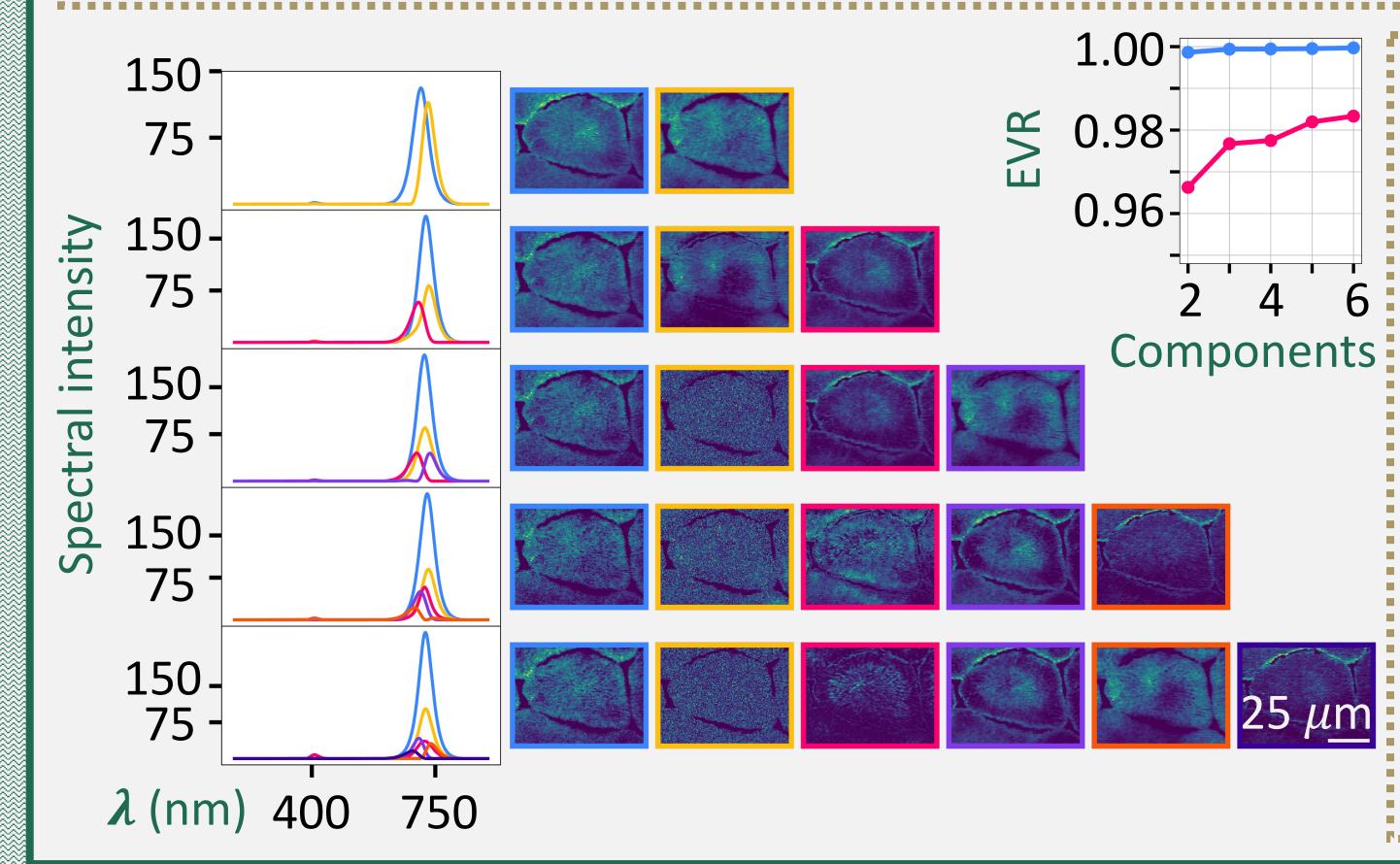
METHODS

- NMF is a machine learning algorithm that produces a parts-based representation of data.¹
- 1 complex matrix is decomposed into 2 matrices of lower rank.
- Right: Wide-field HP cell (top), HP grain boundary (bottom)



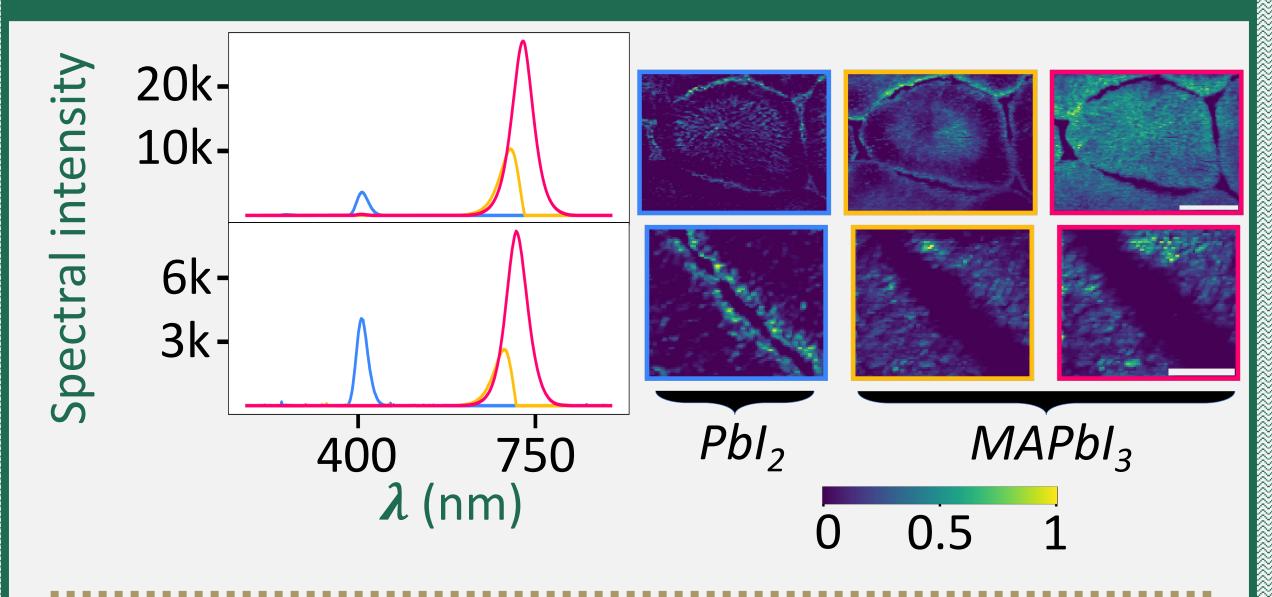
 λ (nm) Original : Denoised

After testing 20+ filter combinations on various spectral signatures, subtracting background and applying a median filter best improved data quality



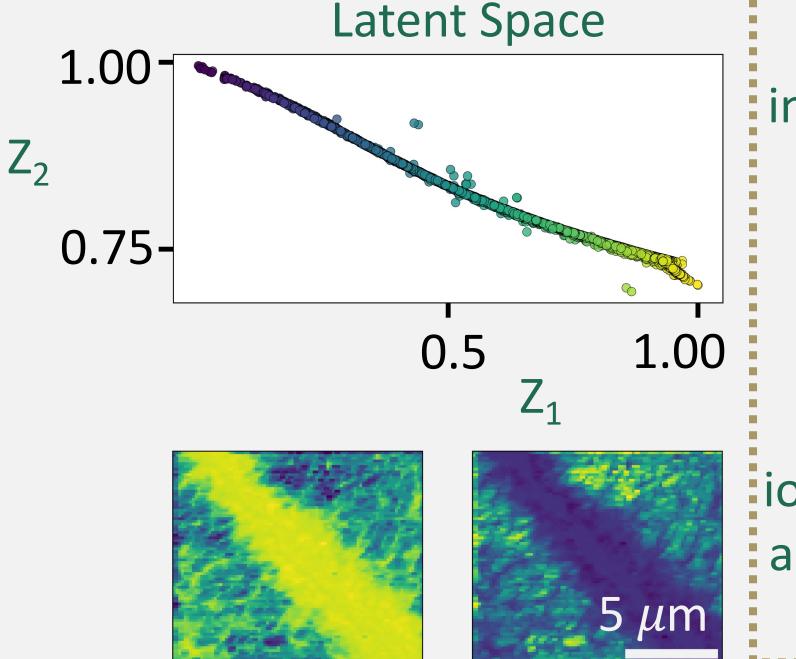
- Blind NMF with 2 to 6 components and explained variance (EVR) suggest 3 components are sufficient
- We enforced sparseness (degree to which a vector is populated by zeros) on the loss function to varying amounts

RESULTS AND DISCUSSION



- 3-component NMF with high spectral sparseness at 200 iterations decomposes the perovskite and lead iodide signatures into separate components.
- HP degrades into lead iodide at grain boundaries where it has higher exposure to humidity.

FURTHER STUDIES



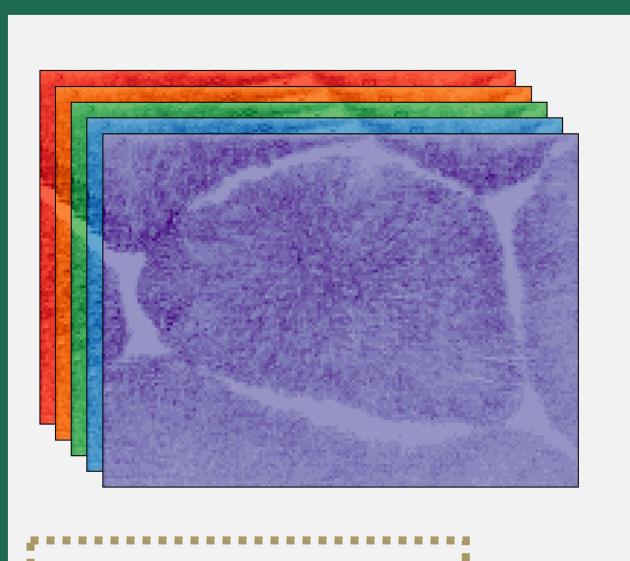
Preliminary investigations using a **variational** autoencoder revealed inverse correlations between lead iodide presence (Z₁) and HP dominance

REFERENCES

Lee, Daniel D., and H. Sebastian Seung. "Learning the Parts of Objects by Non-Negative Matrix Factorization." Nature 401, no. 6755 (October 1999)

ACKNOWLEDGEMENTS

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In CL, A beam of electrons excites the atoms in the HP which emits photons to be directed by a

hyperbolic mirror into a chargecoupled device (CCD).

Hyperspectral datasets of

HP were acquired via scanning electron microscopy (SEM) and cathodoluminescence (CL) spectroscopy, a powerful tool for mapping materials below the diffraction limit.

