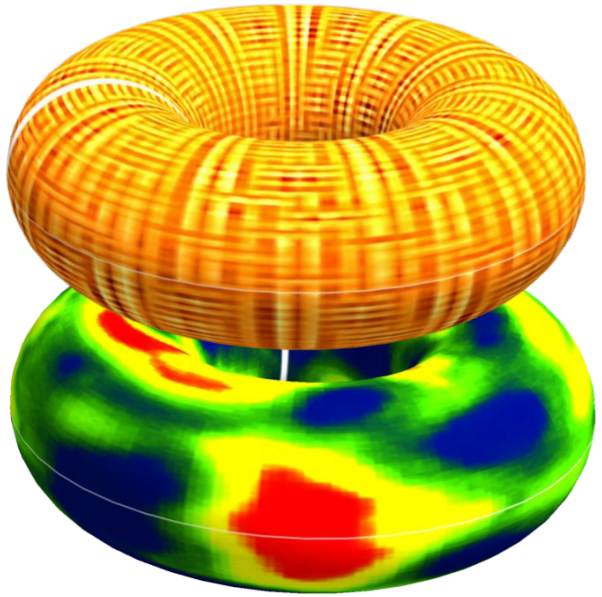
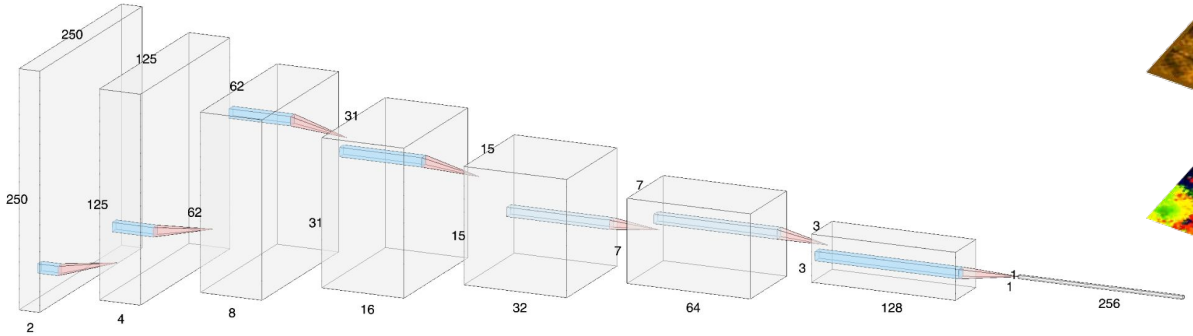
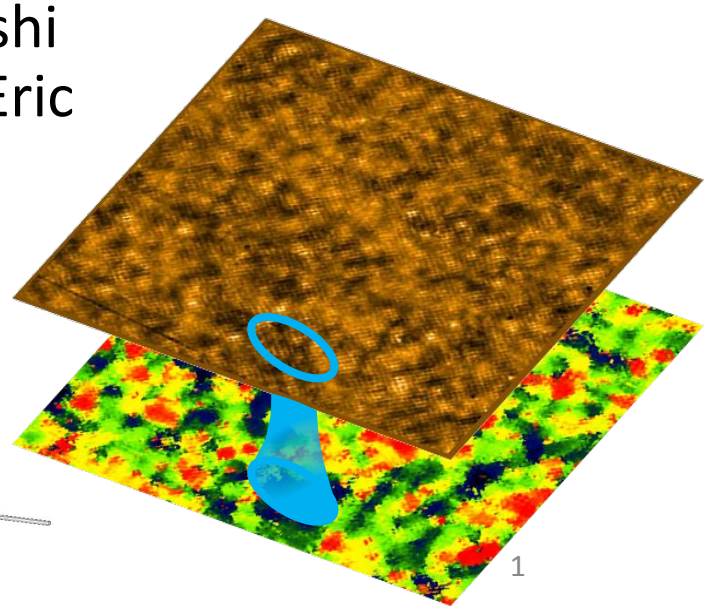
Machine Learning Correlates the Charge Density Wave with the Local Gap in Cuprate Superconductors

By Kaylie Hausknecht

Tatiana Webb, Michael Boyer, Yi Yin, Takeshi Kondo, Tsunehiro Takeuchi, Hiroshi Ikuta, Eric Hudson, Jennifer Hoffman

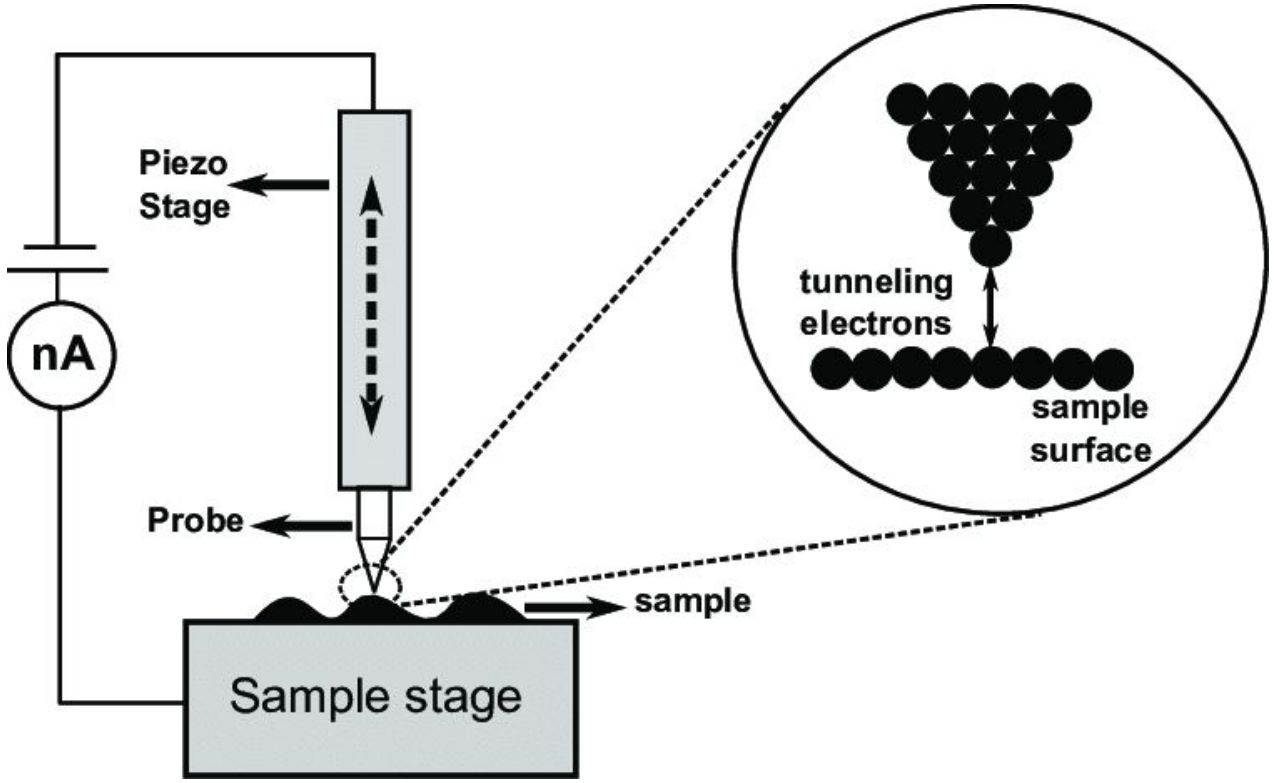






Understanding Disordered Materials

- **CON:** Disorder masks underlying properties
- **PRO:** Disorder can act as an experimental tuning parameter

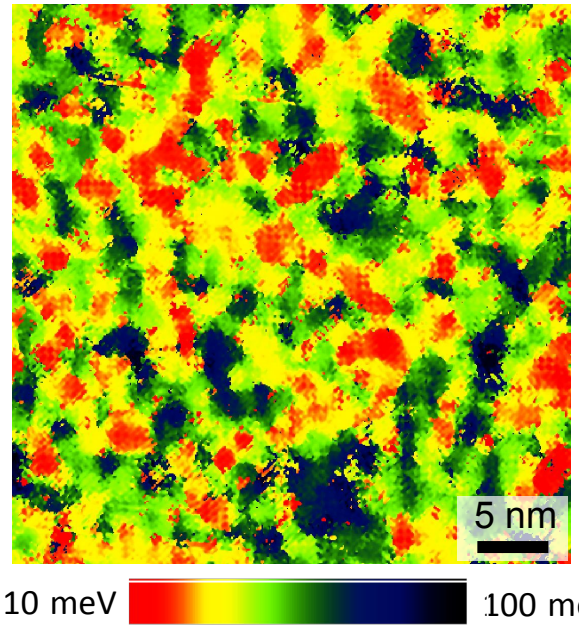


Understanding Disordered Materials

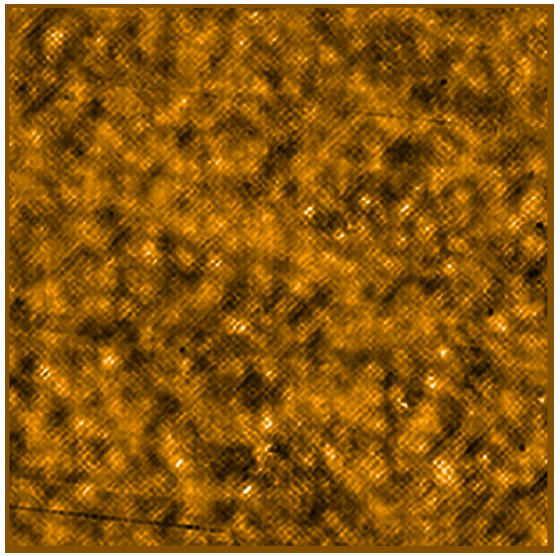
- **CON:** Disorder masks underlying properties
- **PRO:** Disorder can act as an experimental tuning parameter

$Bi_2Sr_2CuO_{6+\delta}$ (Bi2201) Superconductor

X(r)
[gap Δ]



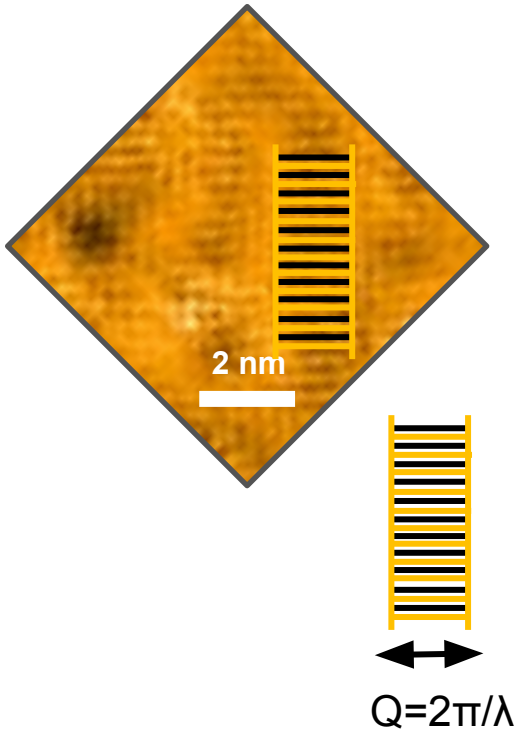
Y(r)
[CDW wavevector q]

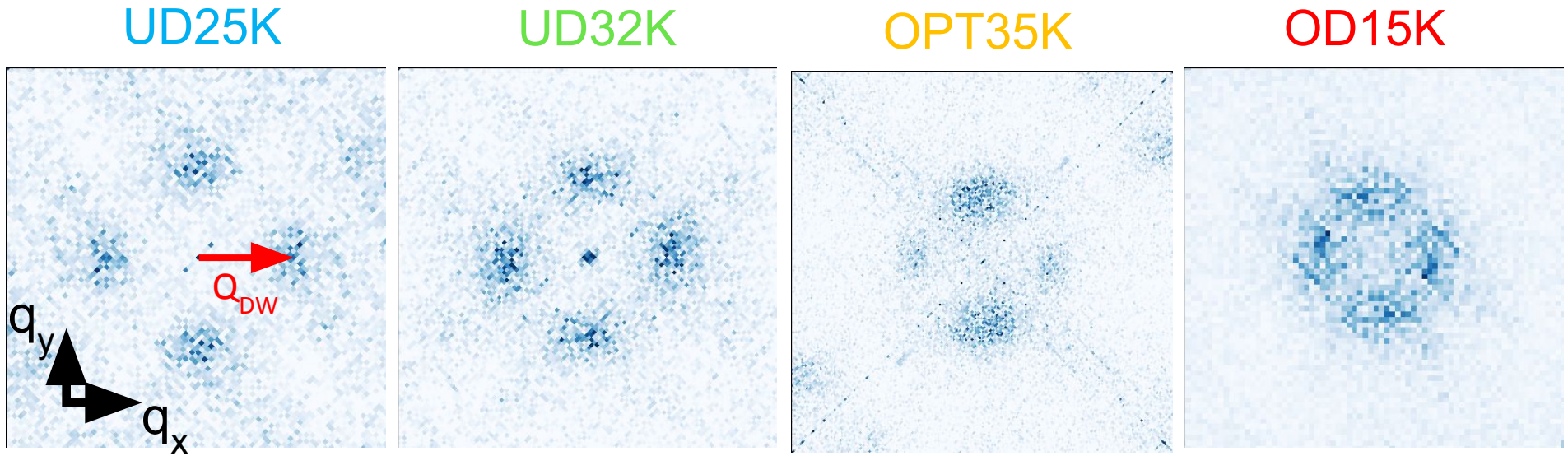


$$Y = f[X]$$

We can look for the function f within a single sample!

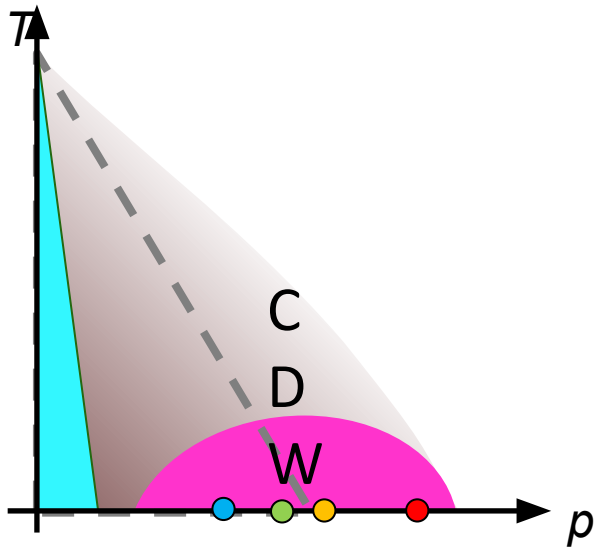
CDW in Bi2201→ Detailed Look

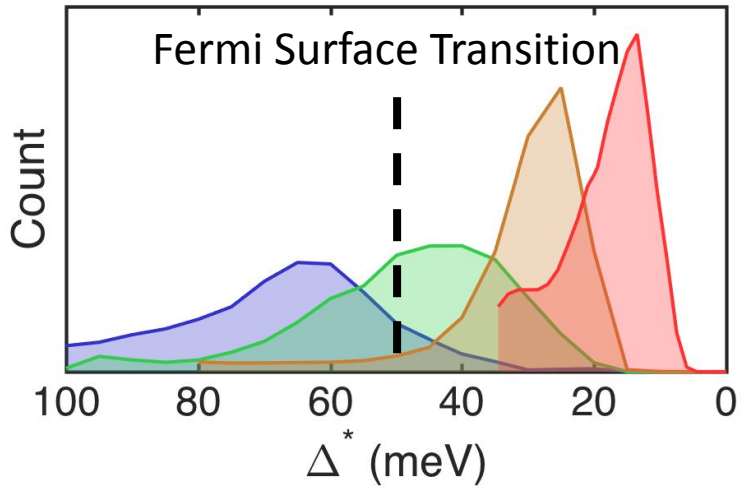




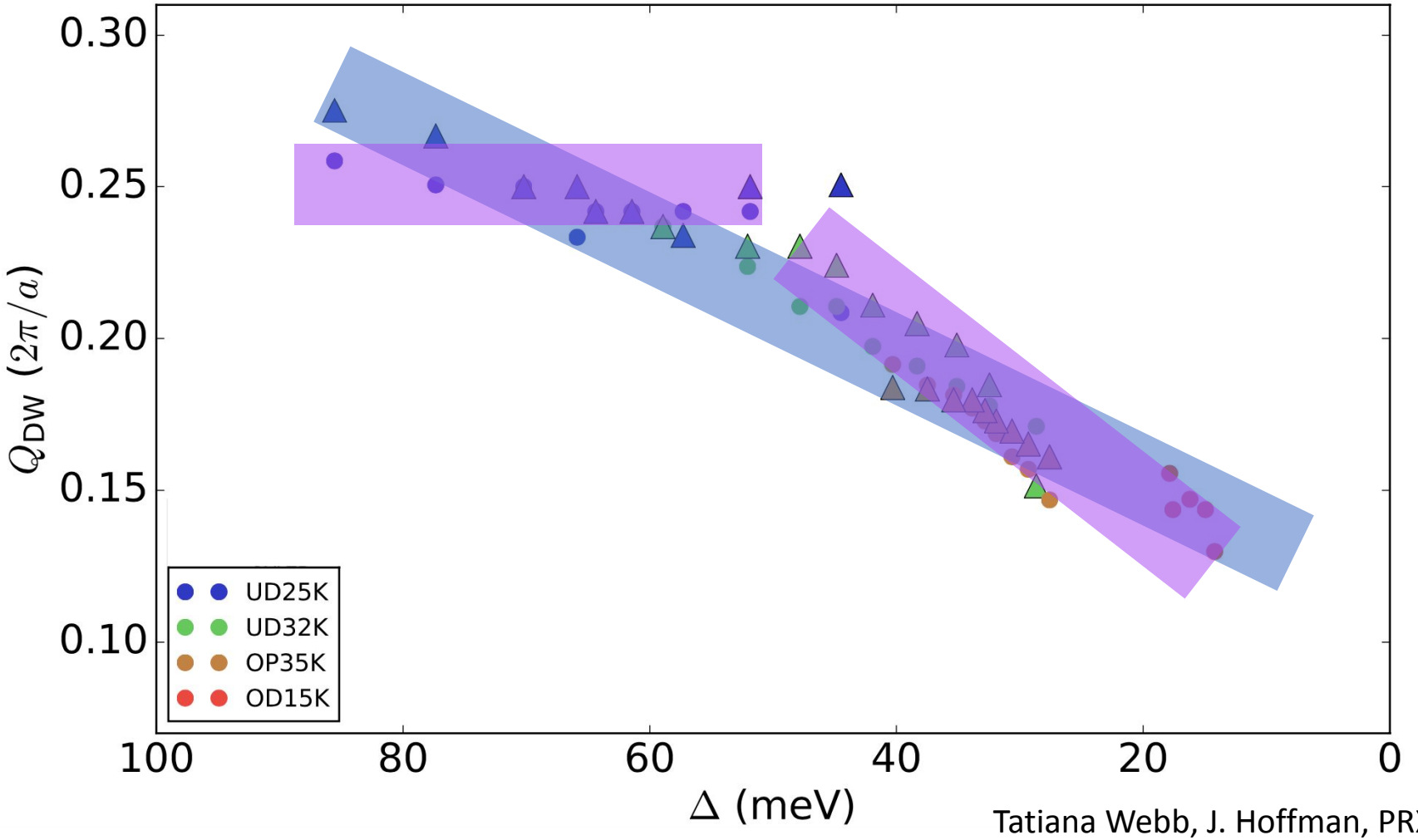
Tatiana Webb, J. Hoffman, PRX 9, 021021 (2019)

Tatiana Webb





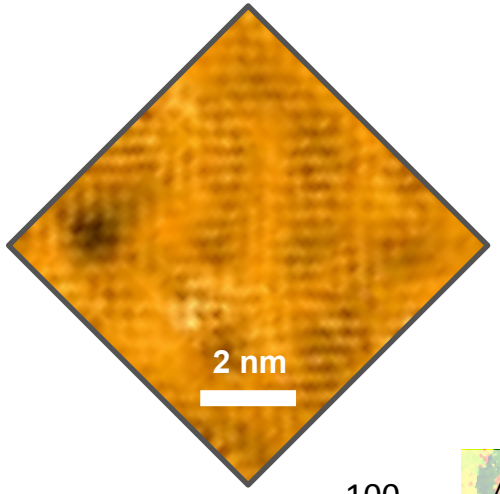
Fourier Masking Technique



Tatiana Webb, J. Hoffman, PRX 9, 021021 (2019)

Losing information from images → Fourier space → points → fitting!

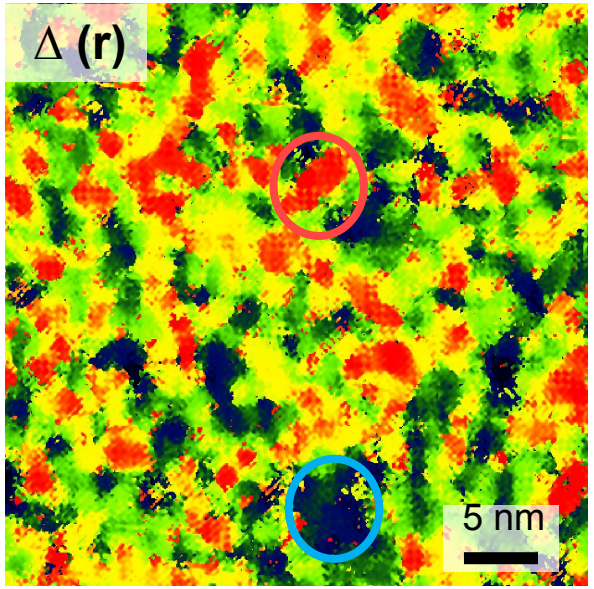
Spatial Variations in Q(Δ(r))

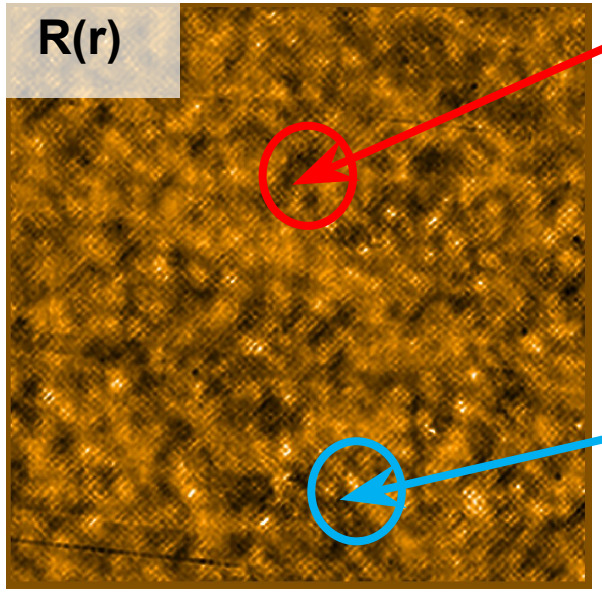


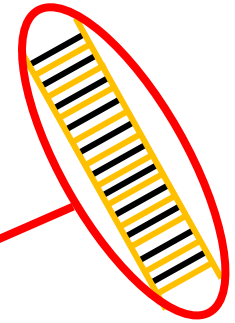
λ=2π/Q

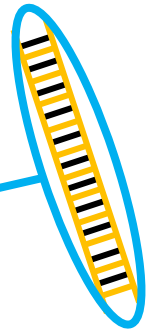
100 meV

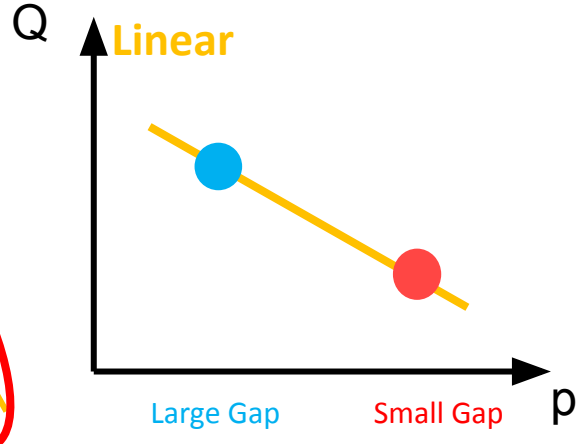
10 meV

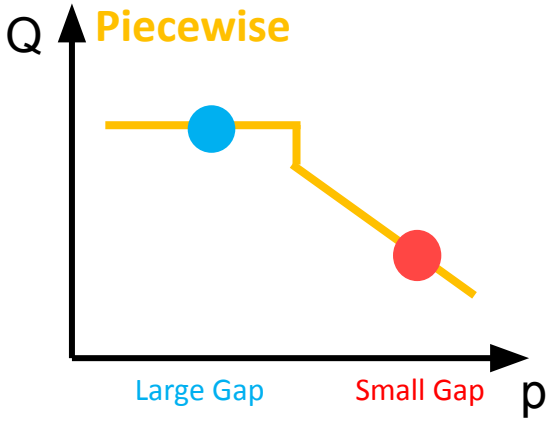






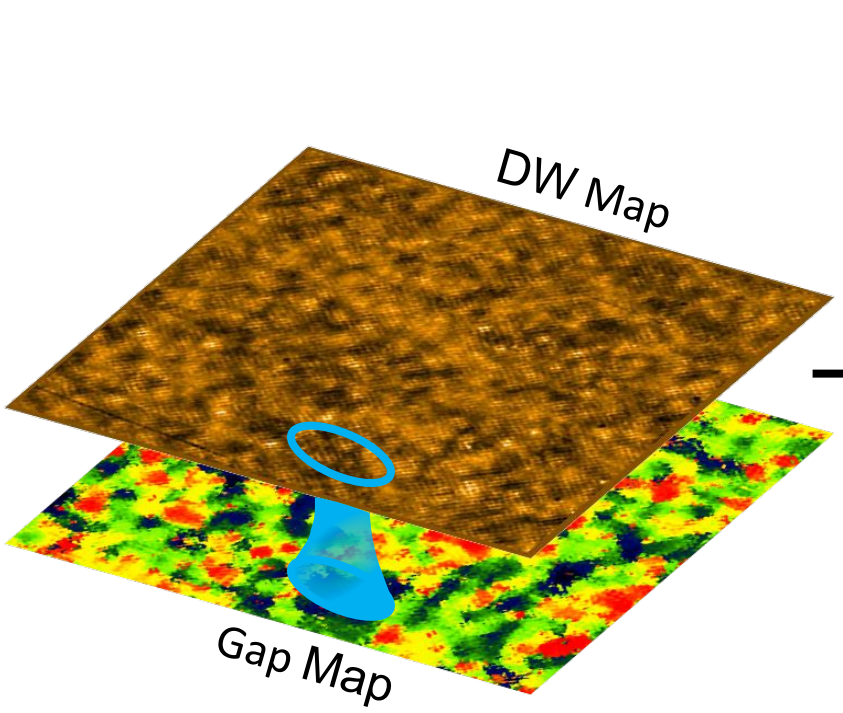


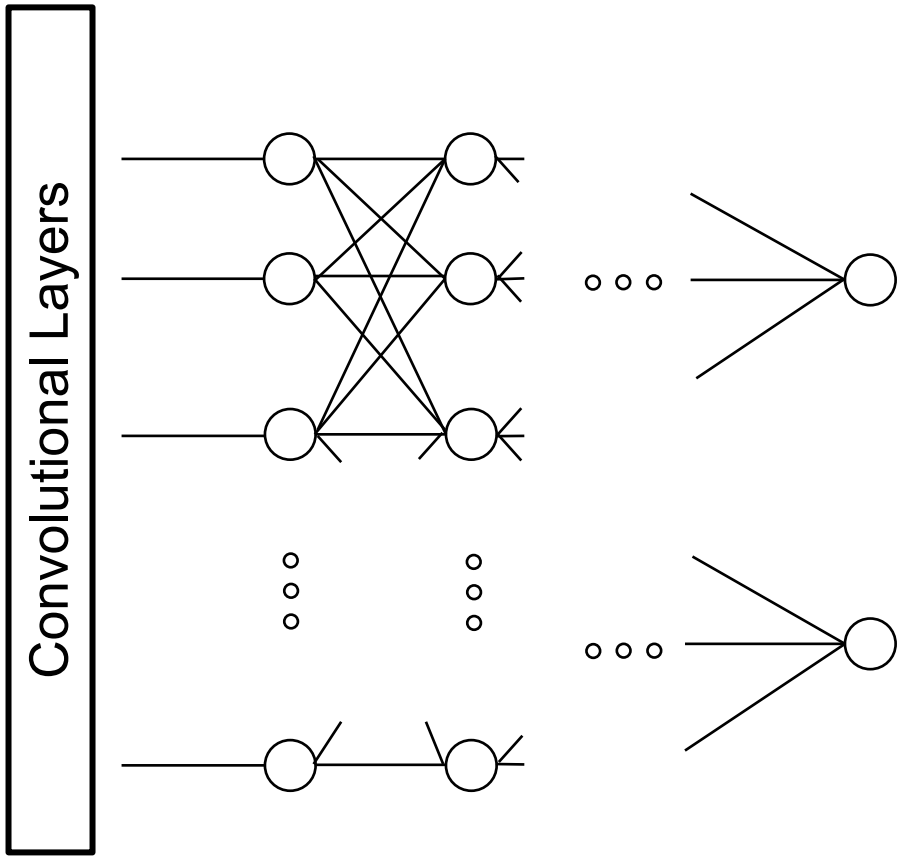


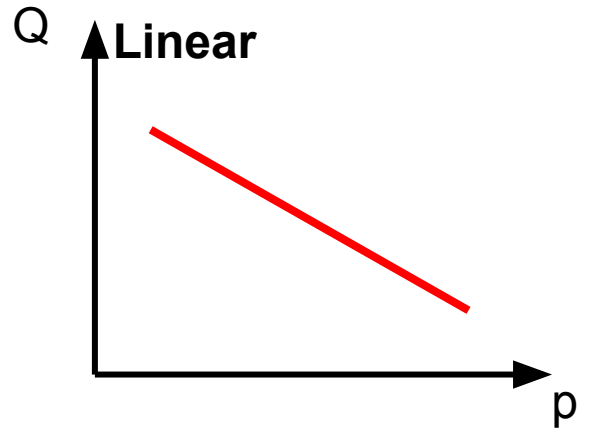


$Q = g(\Delta)$

Neural Network to Detect DW Transition

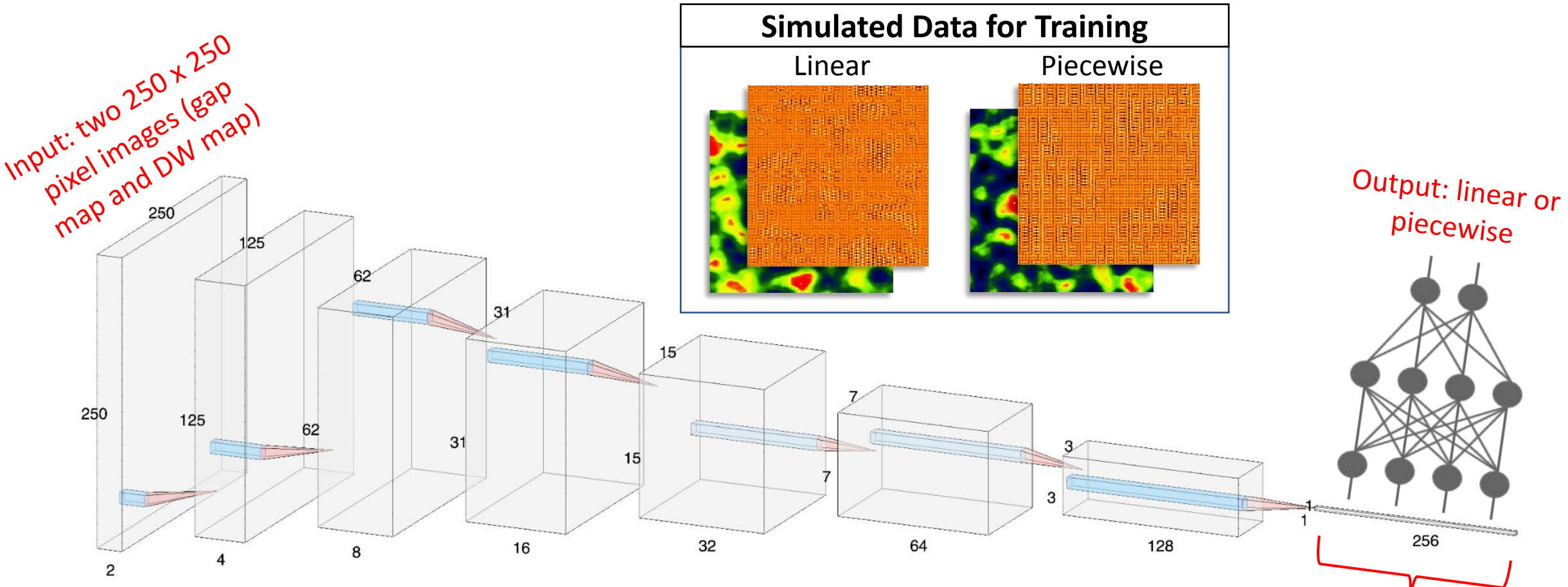




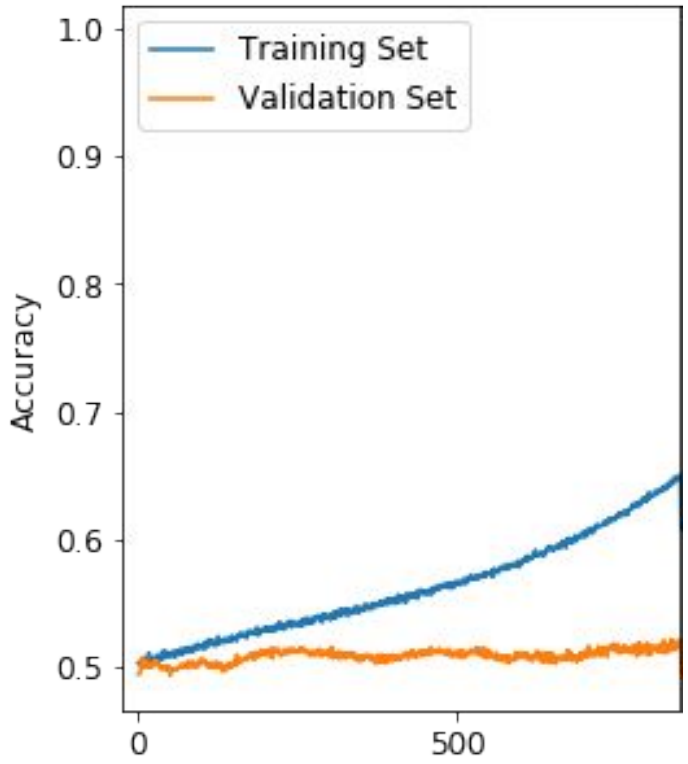


Nielsen, M. (2015). Neural Networks and Deep Learning (Determination Press)

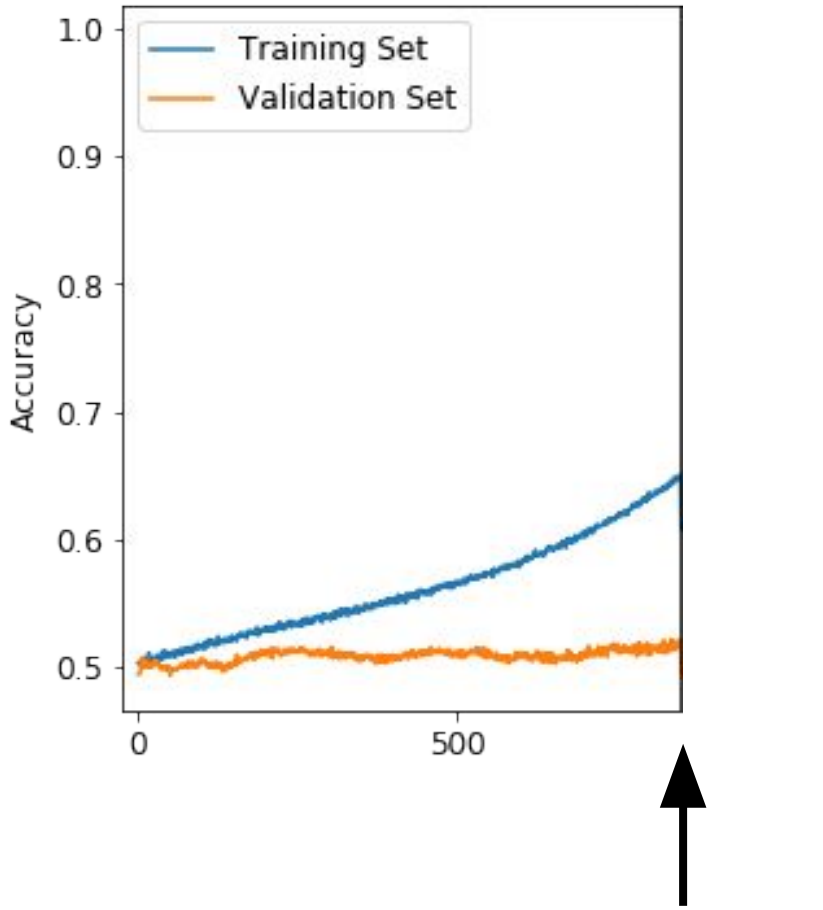
Translationally Invariant Model Architecture



Model Training: Accuracy vs. Validation Accuracy

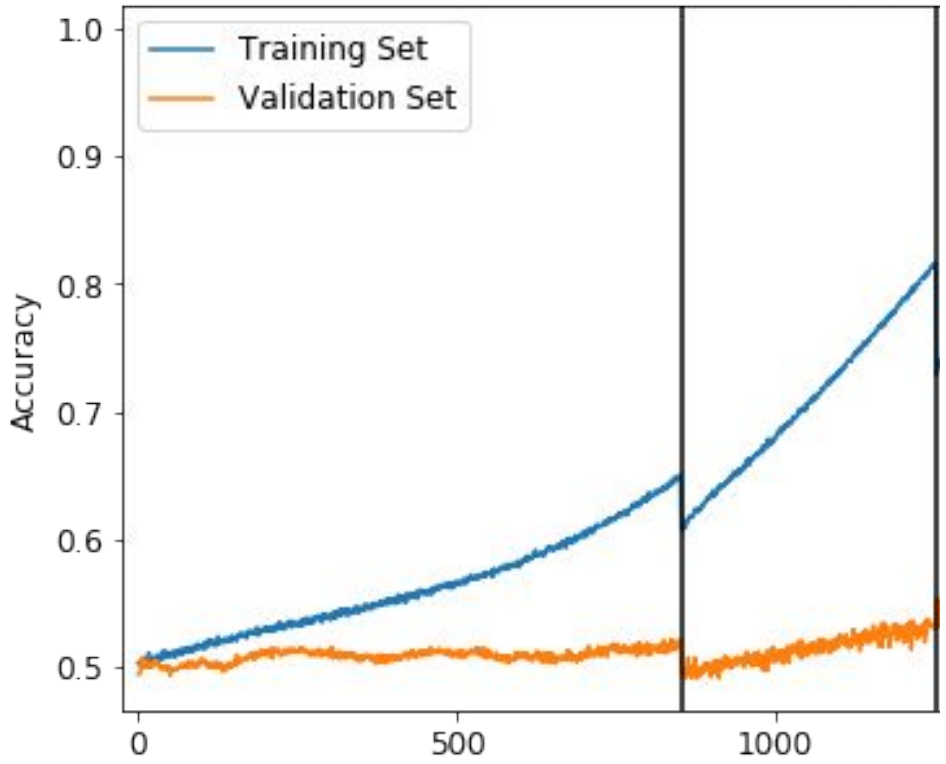


Model Training: Accuracy vs. Validation Accuracy

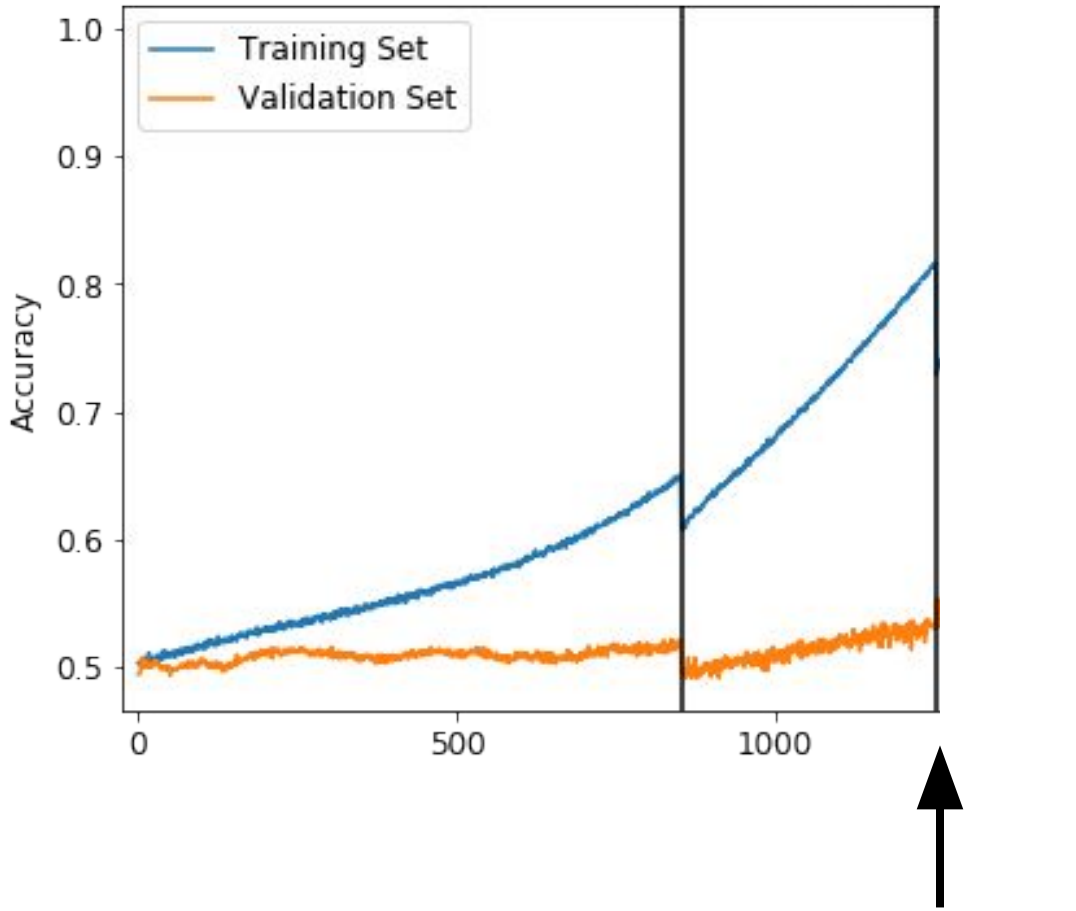


Data Injection

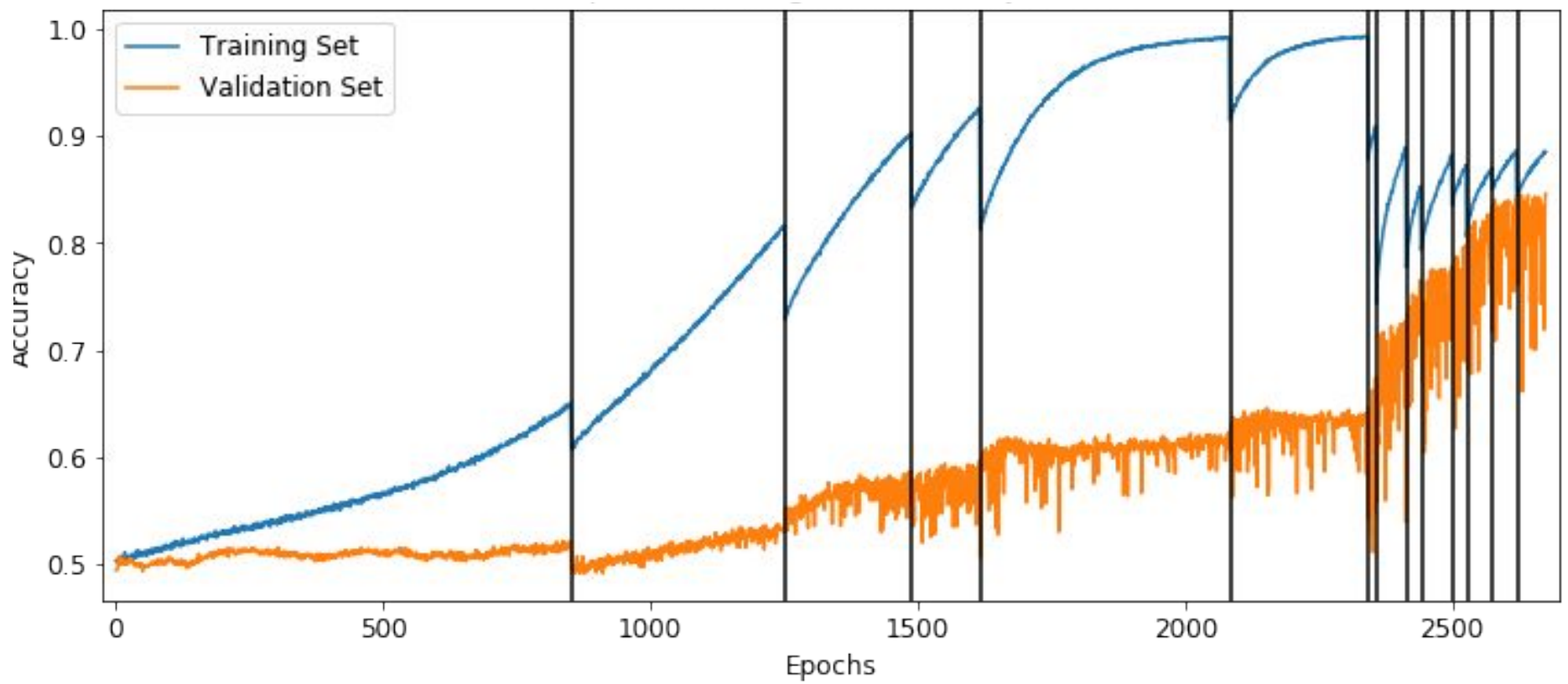
Model Training: Accuracy vs. Validation Accuracy



Model Training: Accuracy vs. Validation Accuracy



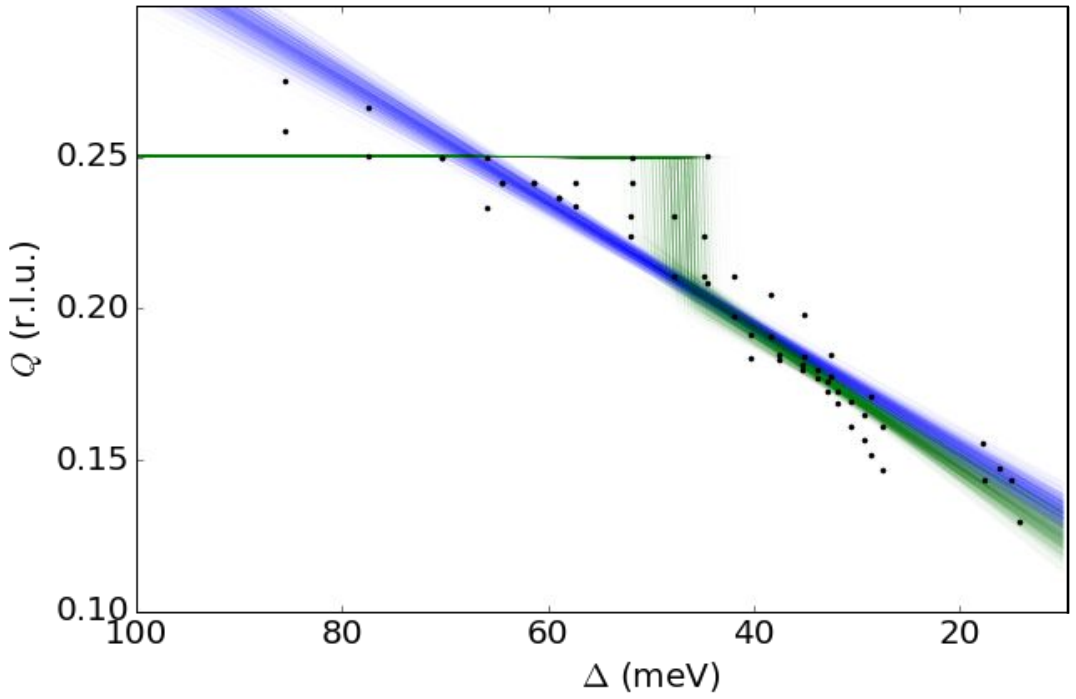
Model Training: Accuracy vs. Validation Accuracy



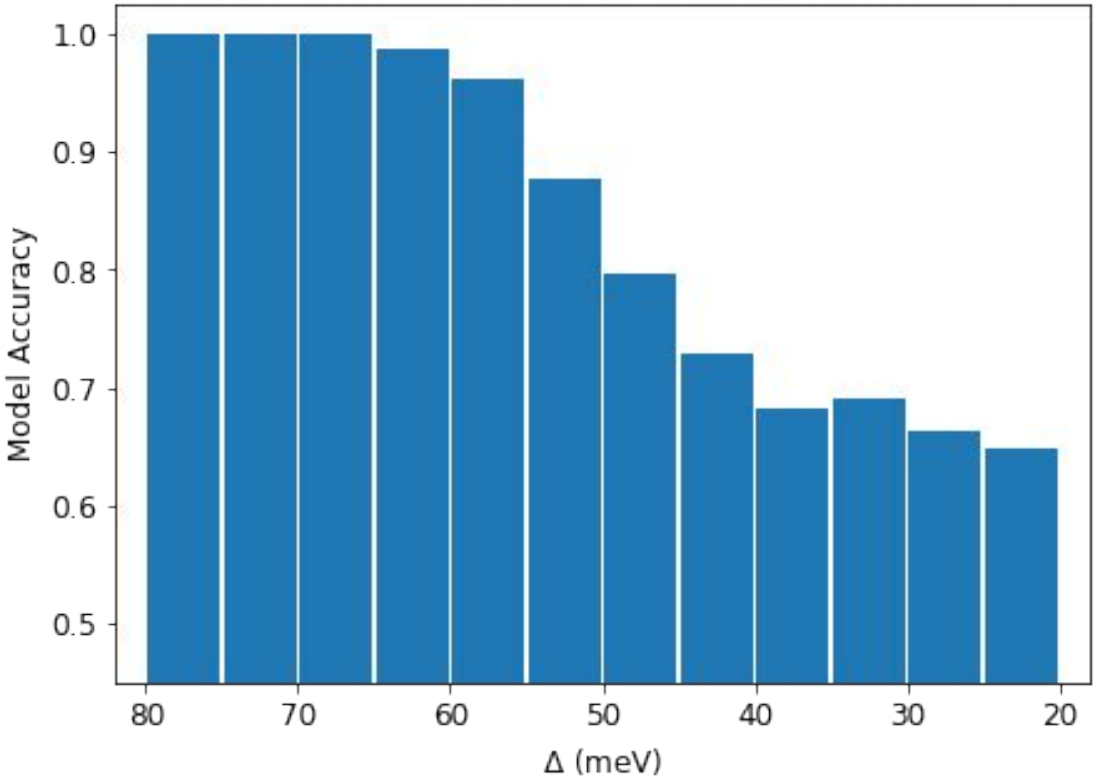
≈ 85% accurate on test data

Accuracy Tracks Hypothesis Overlap

Linear vs. Piecewise Hypothesis

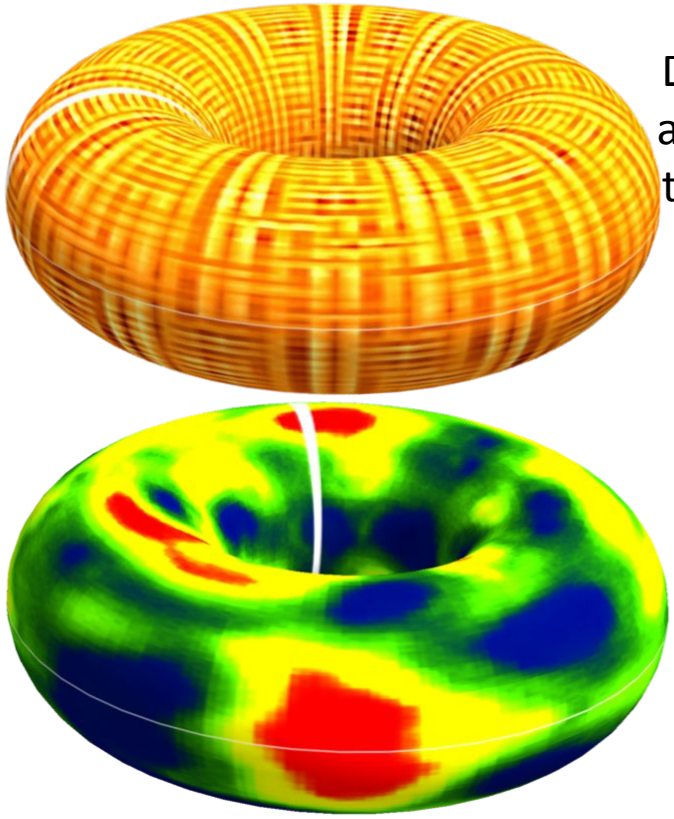


Accuracy Across Gap Range



Simulating Data on a Torus

Periodic Boundary Conditions

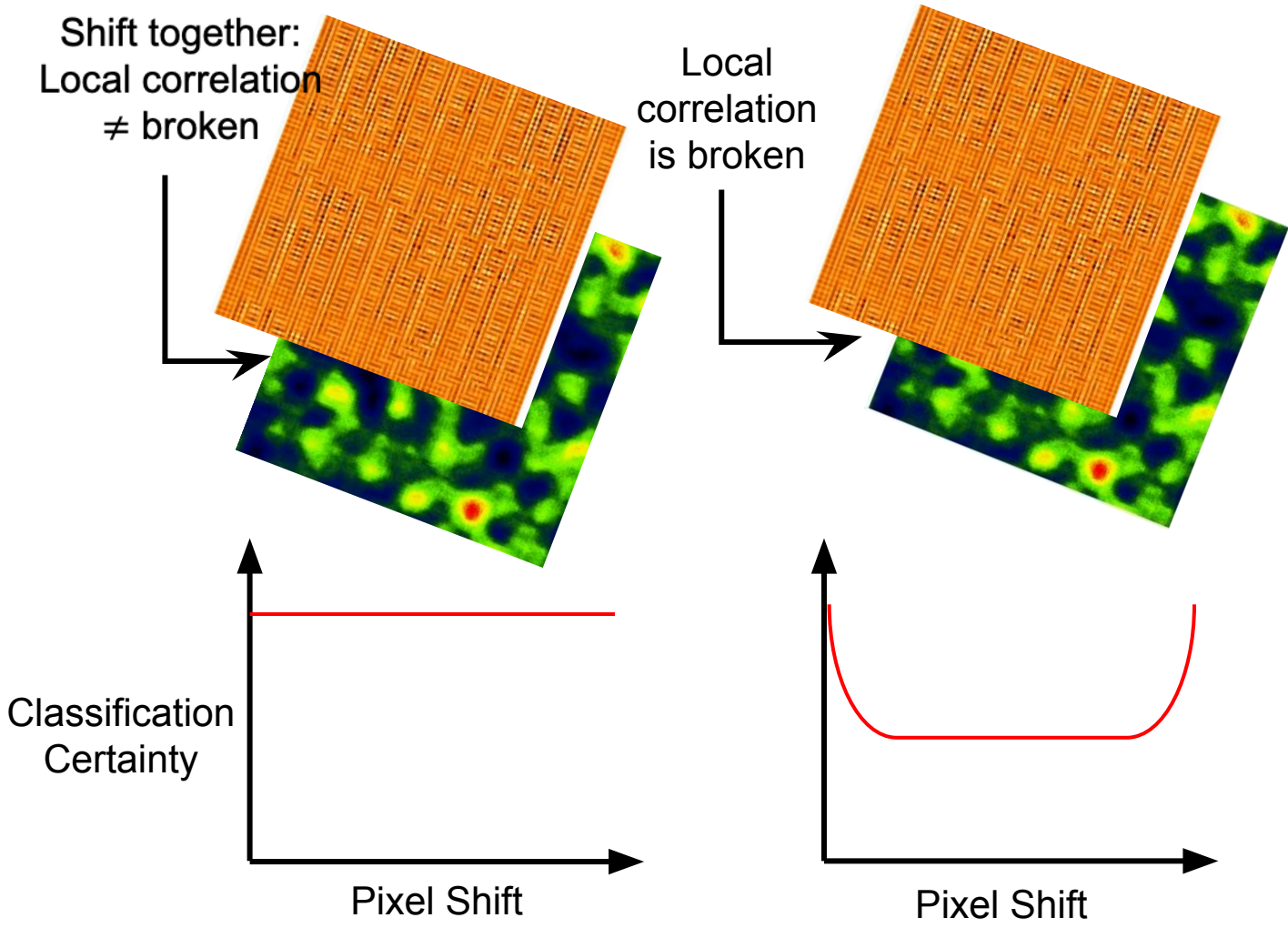


DWs simulated from a gap map by one of the two hypotheses

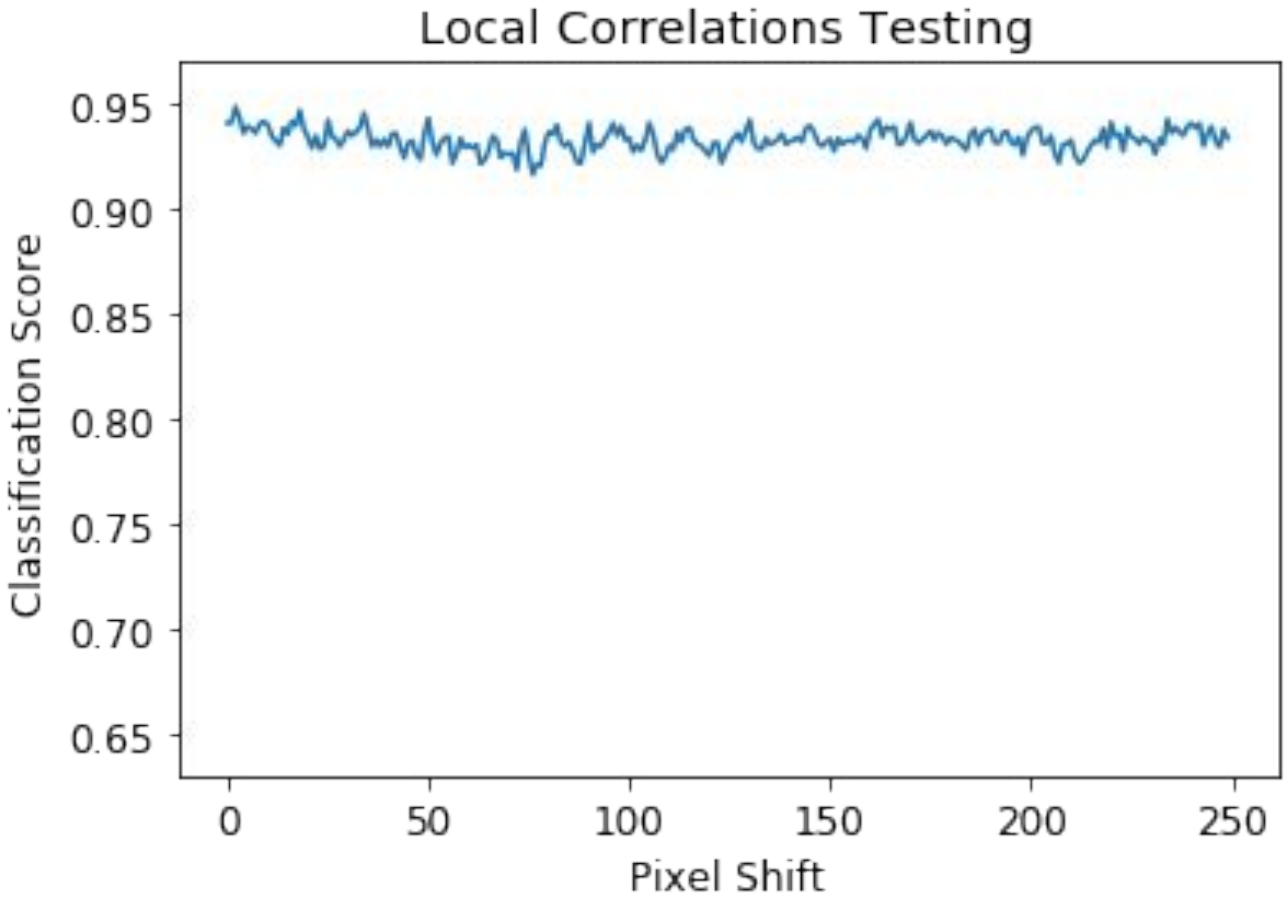
Generated by smoothing Poissonian noise, binning, and sharpening edges

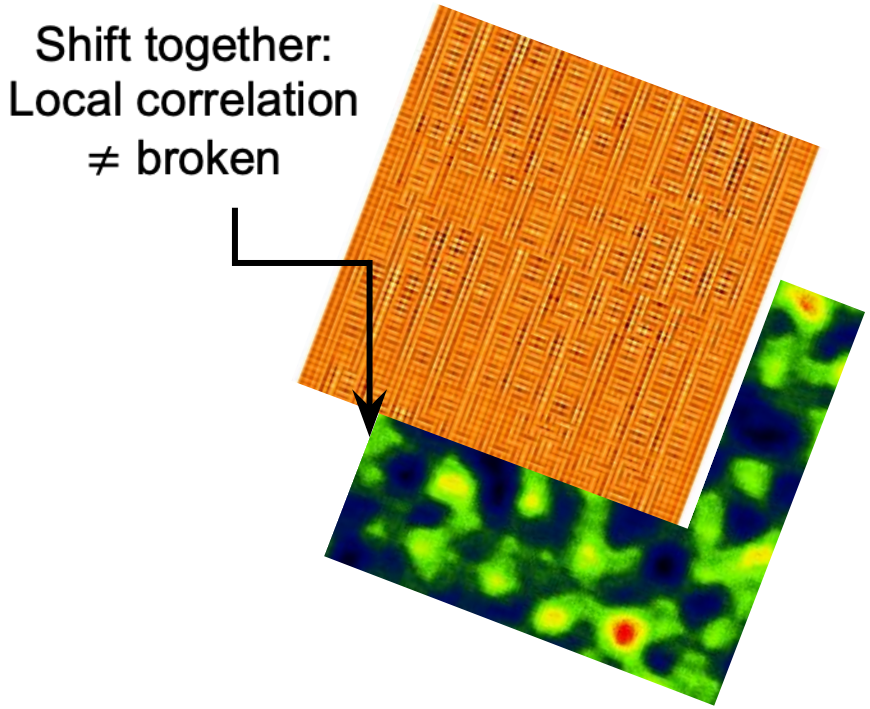
"Mapping Photographic Images to 3D Surfaces"
http://demonstrations.wolfram.com/MappingPhotographicImagesTo3DSurfaces/
Wolfram Demonstrations Project

Ideal Translation Interpretability Tests

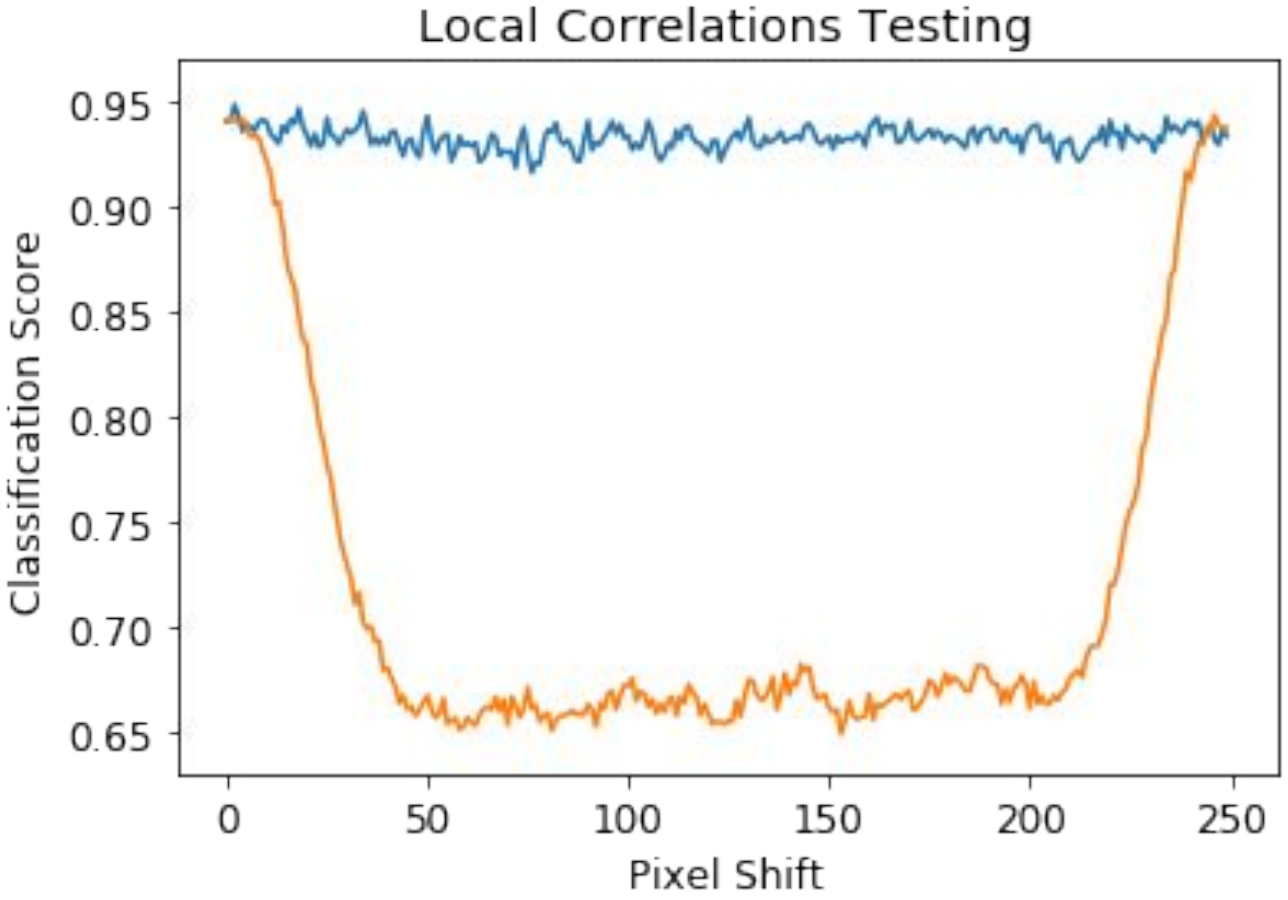


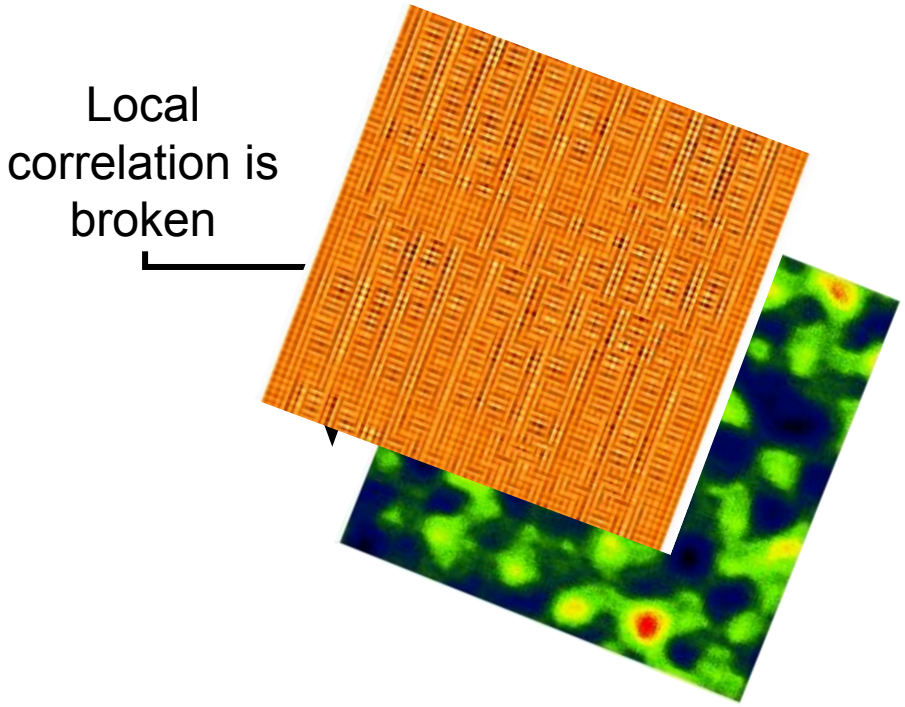
How Certain is the Model in its Classifications?





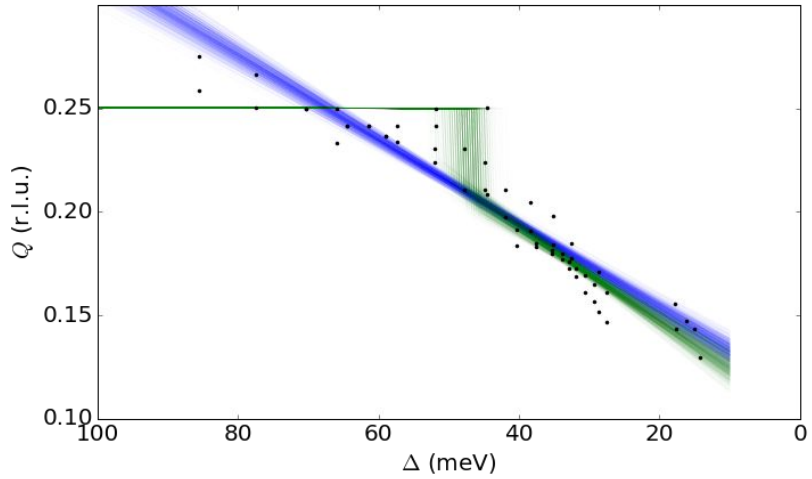
Is the Model Learning Local Correlations (i.e. F(X)=Y in 2D)?

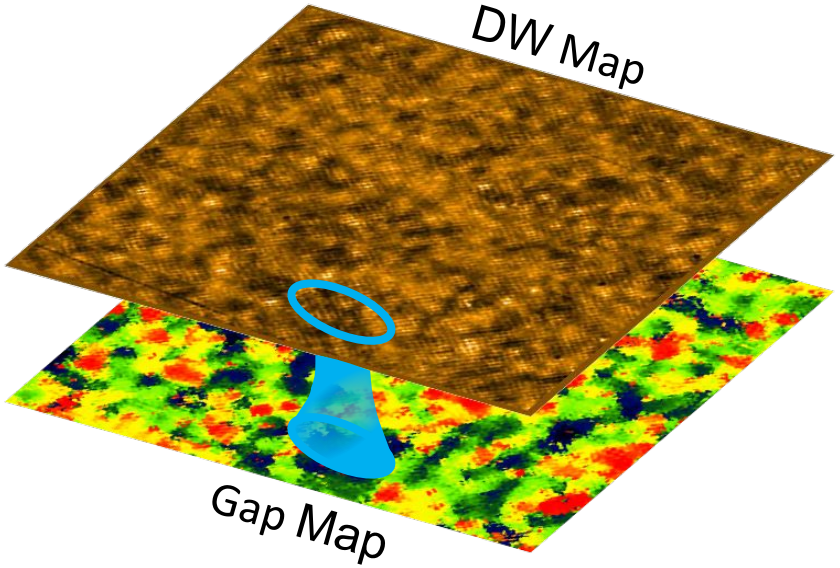




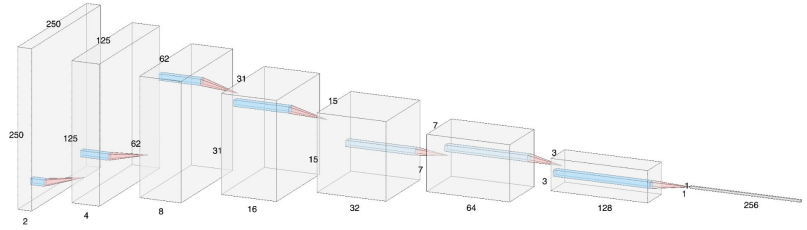
Conclusions

Proved: Local learning to find f(X)=Y, within two 2D images

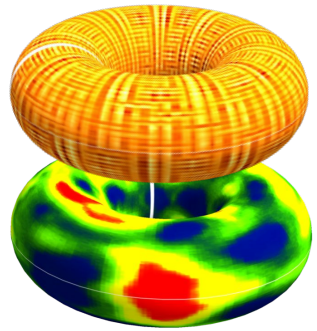




- Convolutional neural networks
  → pooling induces translational invariance



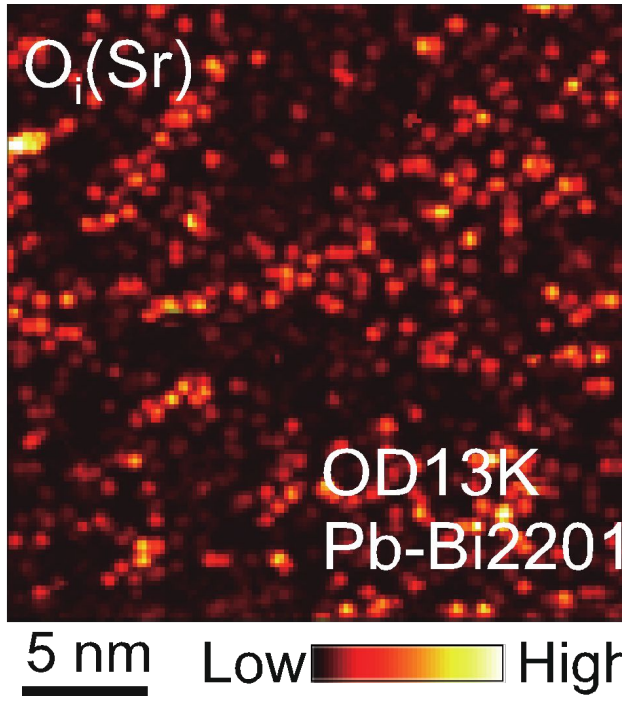
- Synthetic data on a torus
  → shift interpretability test



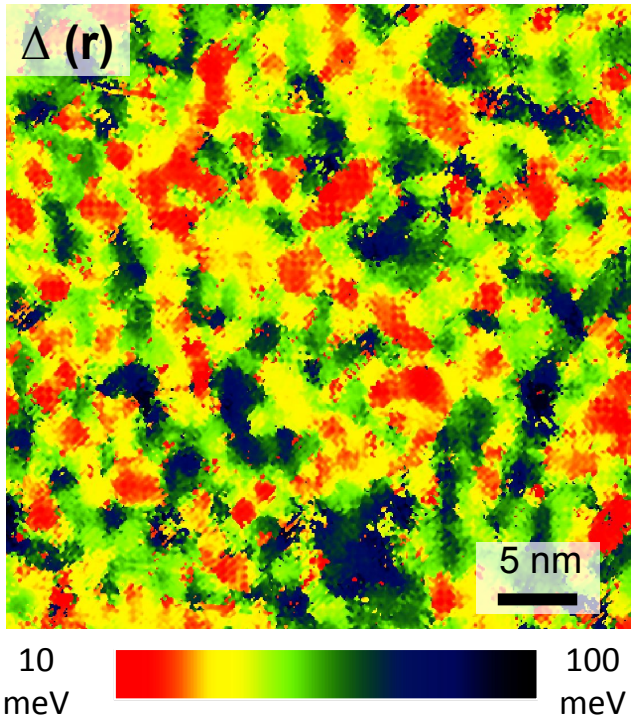
Next steps:

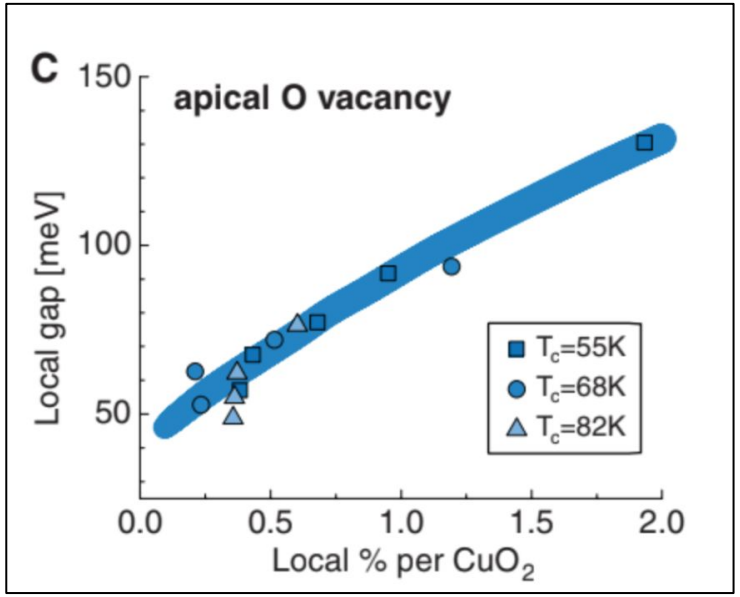
- Predictions on real data

Bi2201: Local Doping Controls Electronic Inhomogeneity



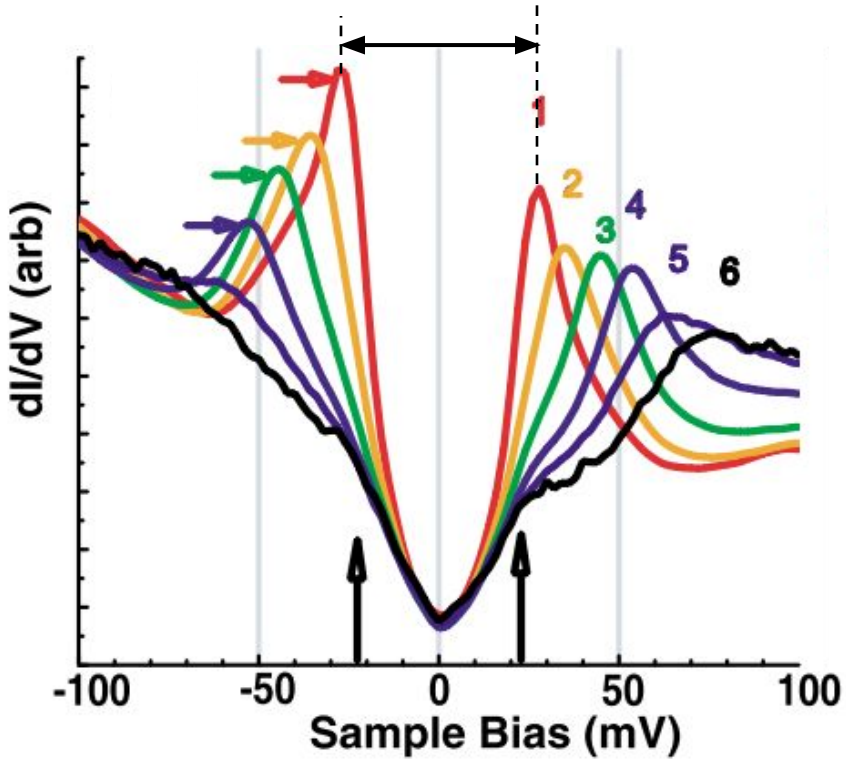
Fei Sci. China Phys. Mech. Astron. 61, 127404 (2018)



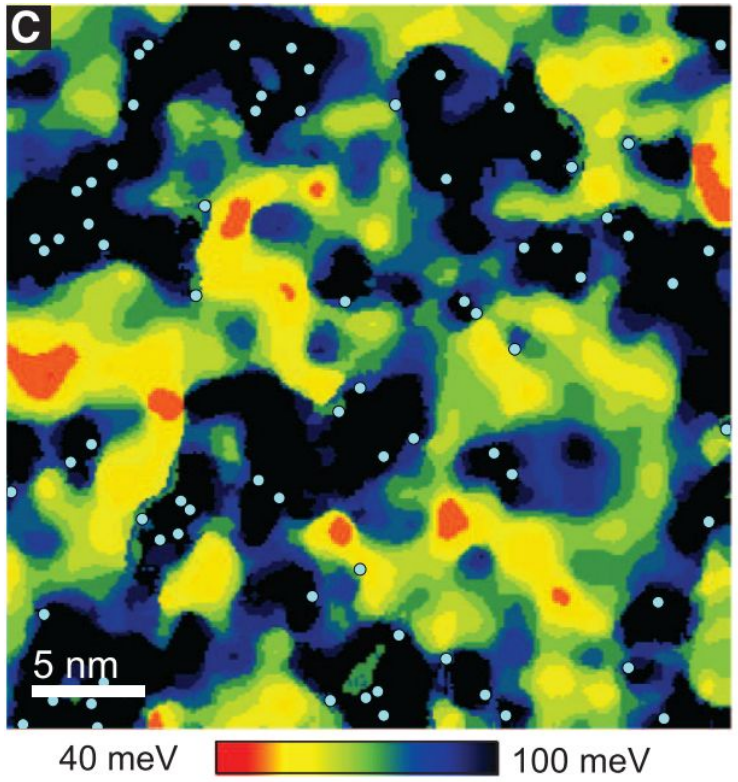


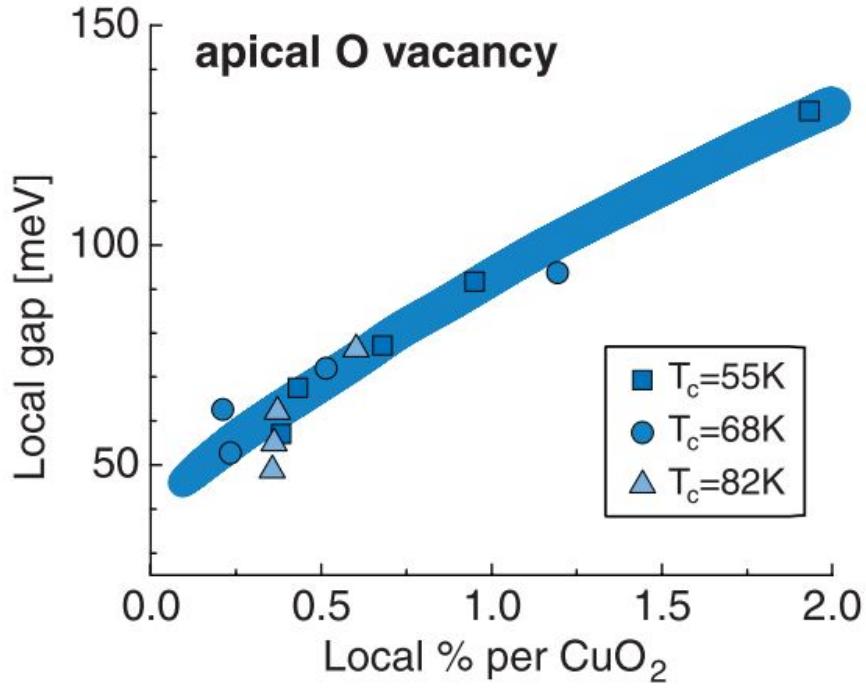
Zeljkovic…Hoffman 337, 320 Science (2012)

Bi2212: Local Doping → Electronic Inhomogeneity



McElroy, Hoffman, … Davis
PRL 94, 197005 (2005)



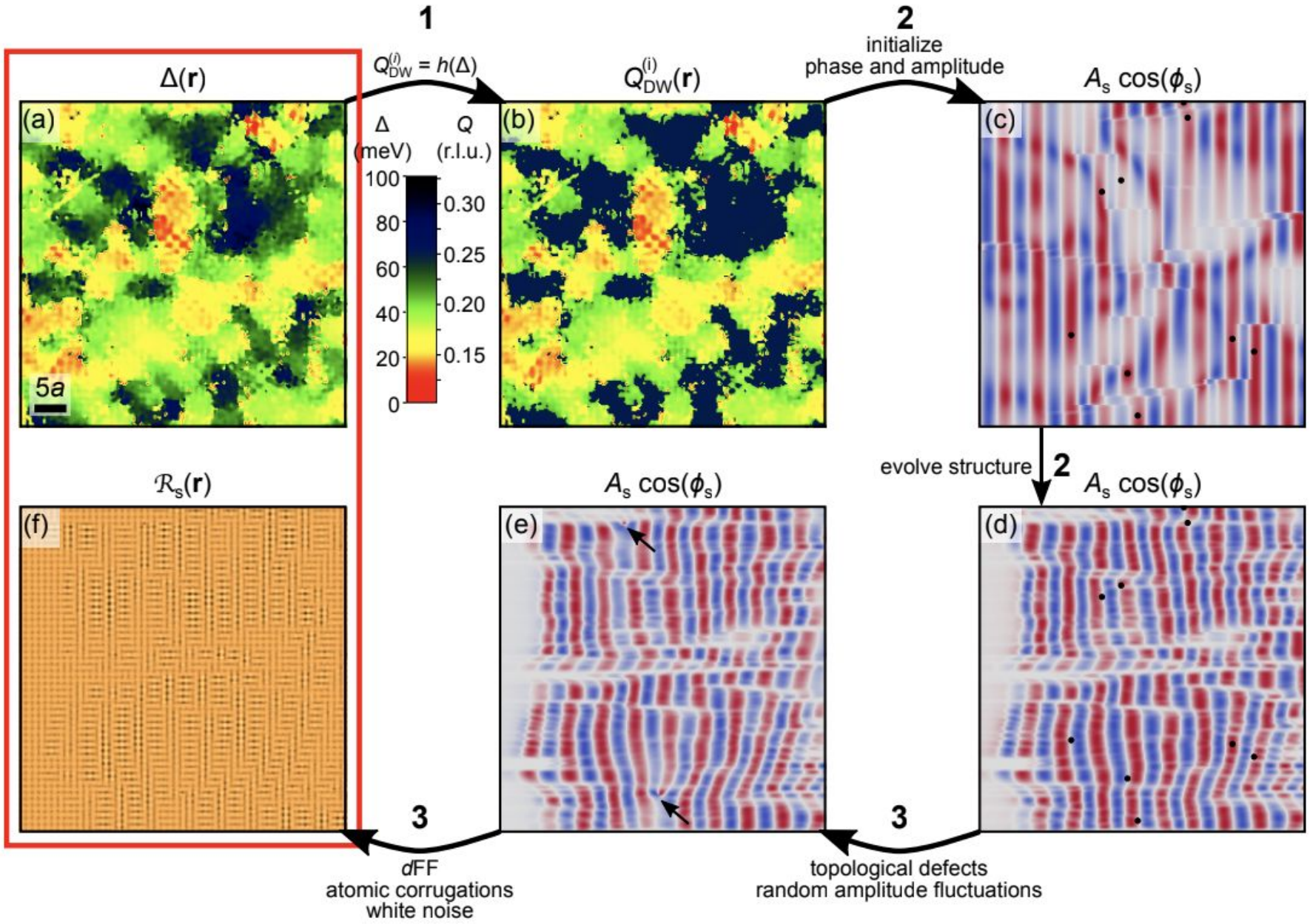


Zeljkovic…Hoffman
Science 337, 320 (2012)

Synthetic Data Simulation

Experimental

Synthetic



Fujita, K., & Hamidian, M et al (2014). Direct phase-sensitive identification of a d-form factor density wave in underdoped cuprates. PNAS, 3026-3032. doi:10.1073/pnas.1406297111

Hamidian, M., & Edkins, S. (2015). Atomic-Scale Electronic Structure of the Cuprate d-Symmetry Form Factor Charge Density Wave. Nature Physics, 59-88. doi:10.1007/978-3-319-65975-6_4