

Classifying Surface Probe Images in Strongly Correlated Electronic Systems via Machine Learning

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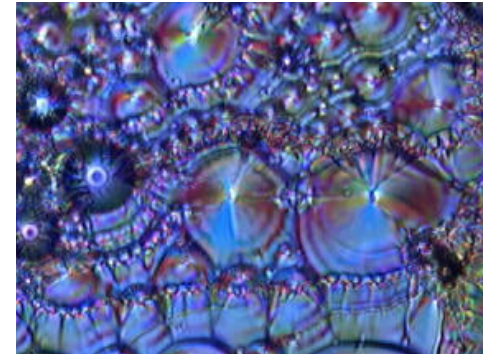


Phys. Rev. Mat. 3, 033805 (2019)



Crystals
Fluids

Liquid Crystals

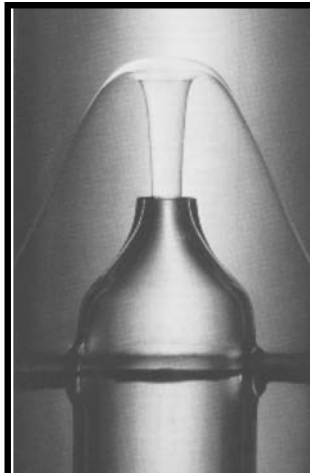


Smectic
Nematic
Hexatic
Cholesteric...

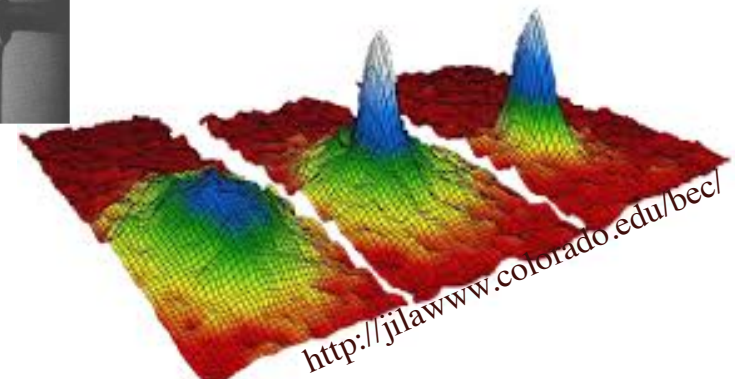


Glass and
Amorphous solids

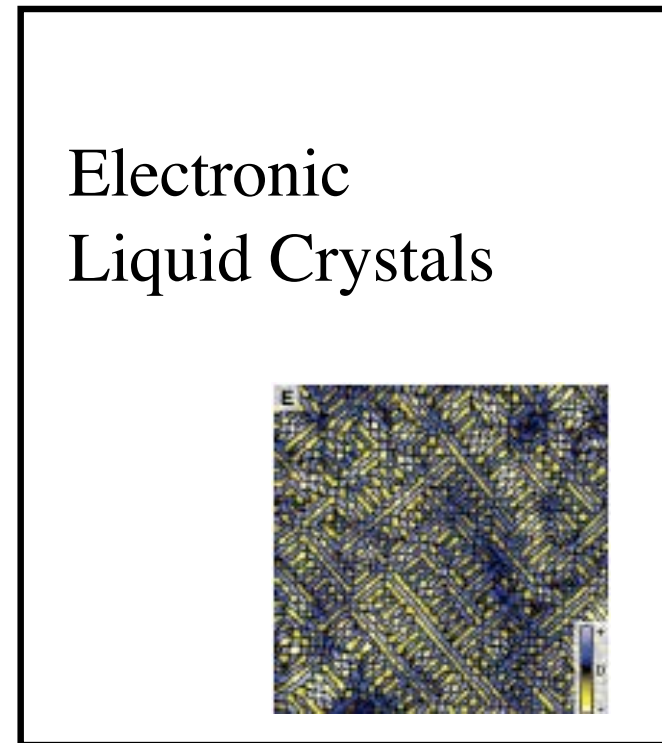
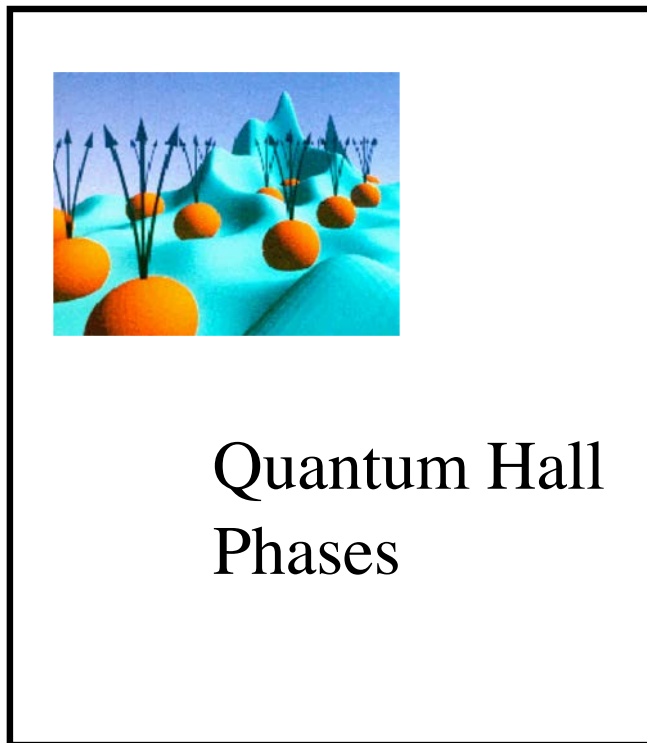
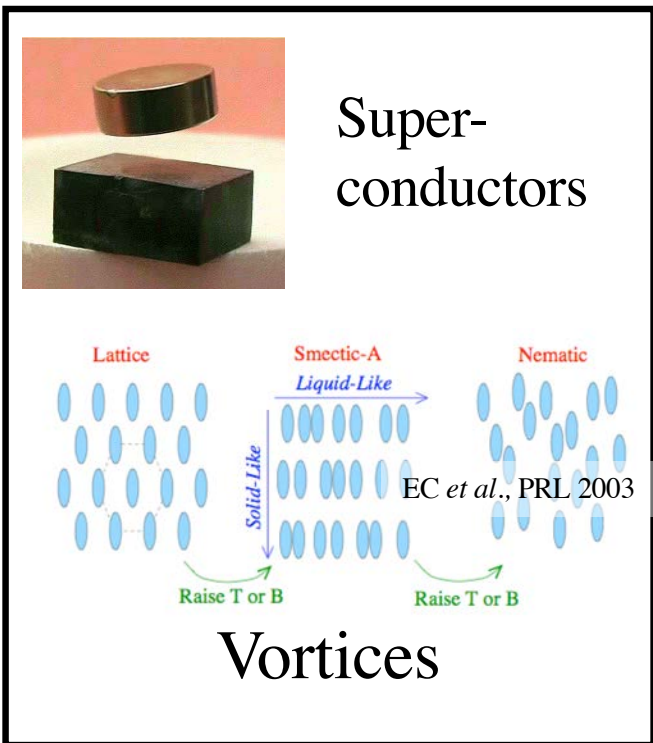
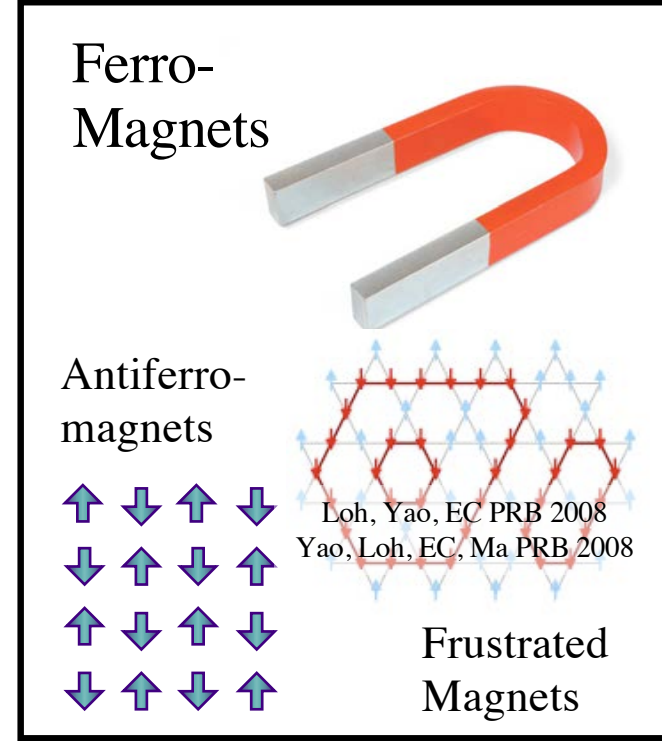
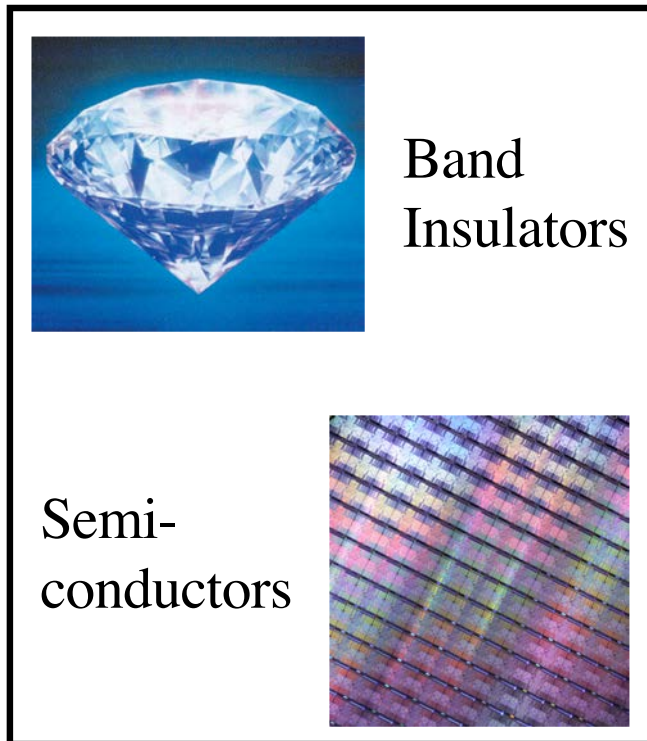
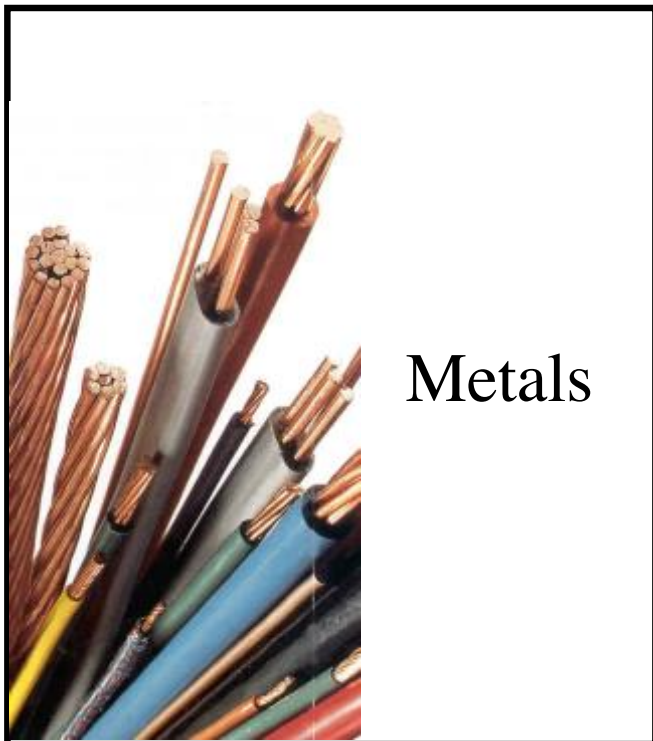
www.dalechihuly.com



Superfluids
and
Bose-Einstein
Condensates



<http://jila.colorado.edu/bec/>

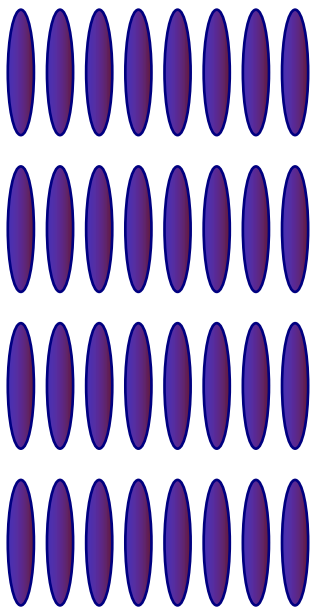


One way we classify phases: Symmetry

By the symmetry of long distance and long time properties

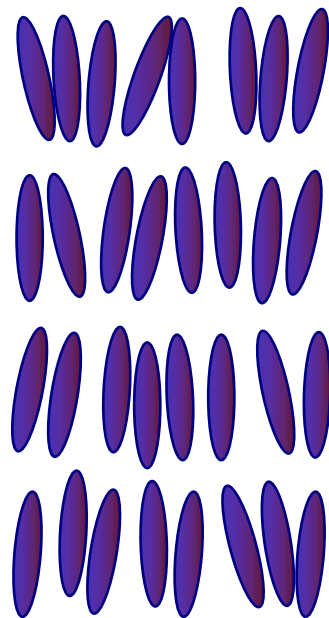
Liquid Crystals

Crystal



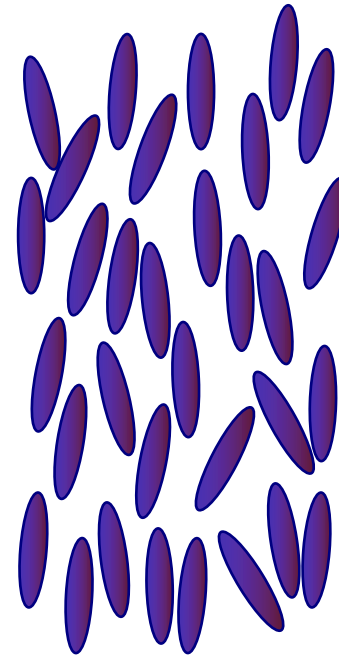
**Periodic
in all directions**

Smectic



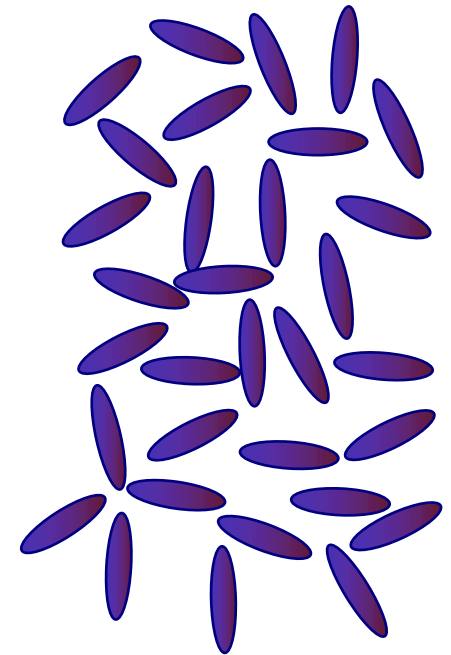
**Periodic
in one direction**

Nematic



Oriented

Liquid



**Smooth
(at long lengths and times)**

Another way we classify phases: Topology

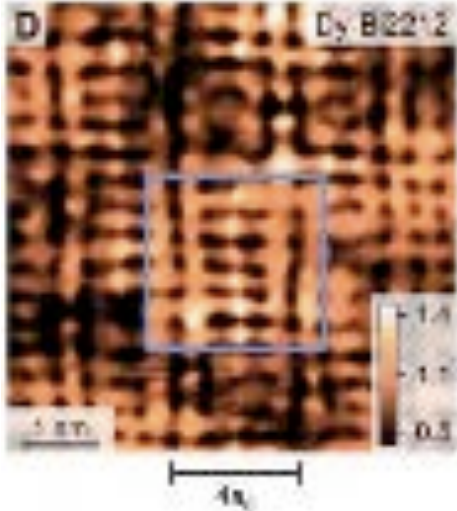


Another way we classify phases: Topology



Is Mesoscale Order Important?

Important nanoscale structure missed by the definition of a phase!



Kohsaka *et al.*,
Science **315**, 1380 (2007)

PROBLEM:

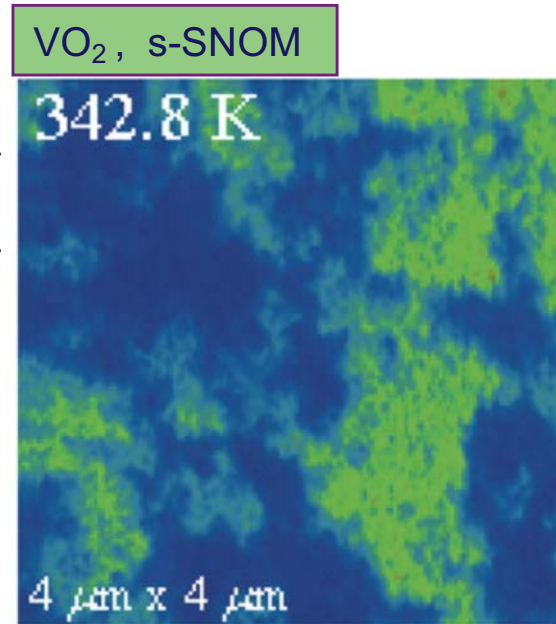
Many theoretical and experimental tools are designed to characterize and detect long distance behavior

Our Solution:

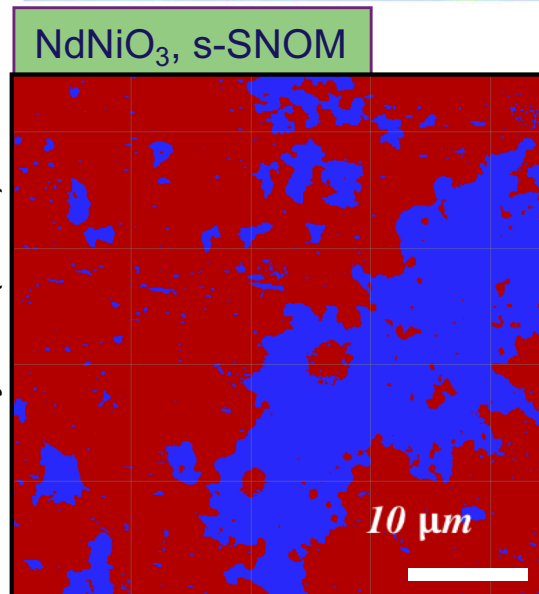
Use the Disorder to our Advantage

Quantum Materials and Disorder

Qazilbash *et al.*,
Science **318**, 1750 (2007)



Post, ... KD, EC, ... *et al.*,
Nature Physics (2018)



Many Degrees of Freedom (DOF)

Spin
Charge
Orbital
Lattice

Strong Correlation + Many DOF

Many Phases Possible
Different Phases Compete

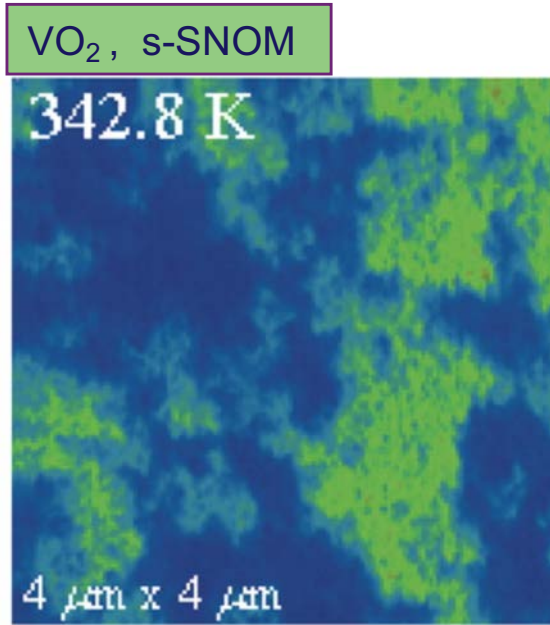
Competing Phases + Disorder

Nanoscale pattern formation
Complexity
Multiple Length Scales

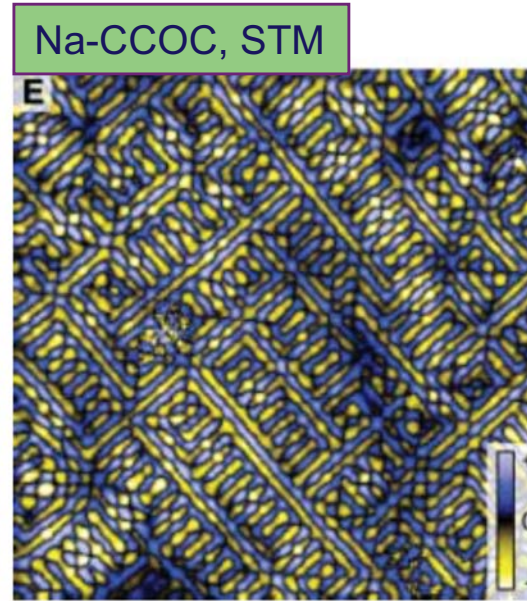
E. Dagotto, Science (2005)

Spatial Complexity in Quantum Materials

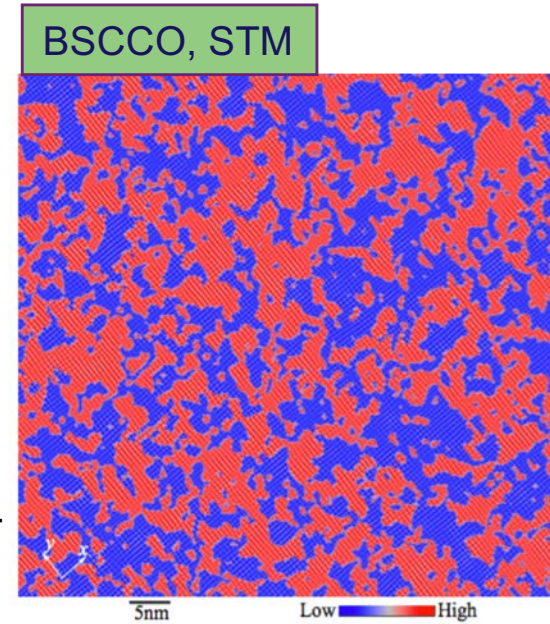
Qazilbash *et al.*,
Science **318**, 1750 (2007)



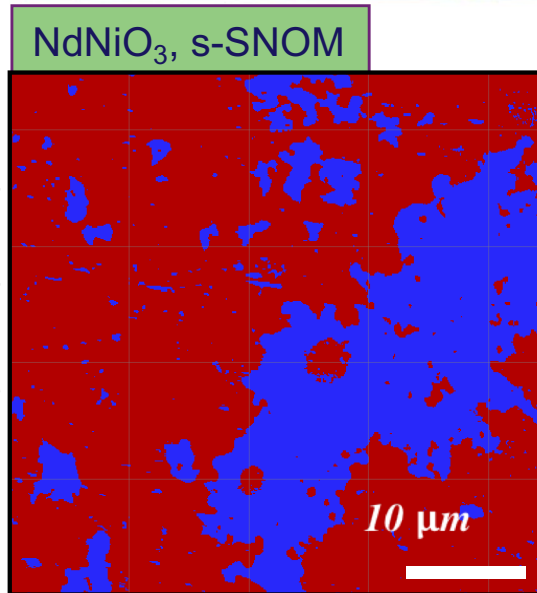
Kohsaka *et al.*,
Science **315**, 1380 (2007)



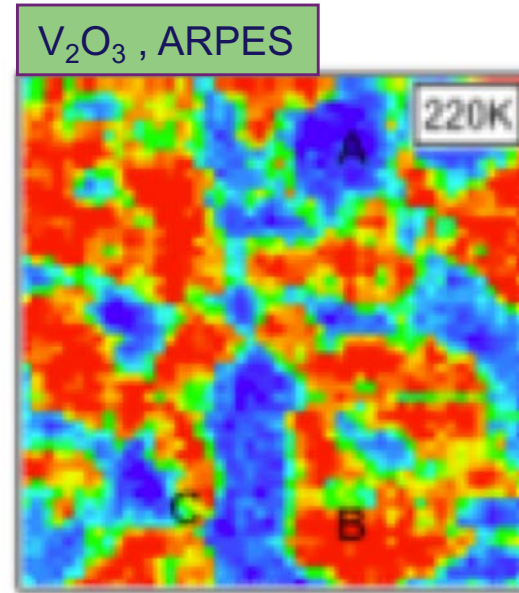
Main, Hoffman, *et al.*,
unpublished



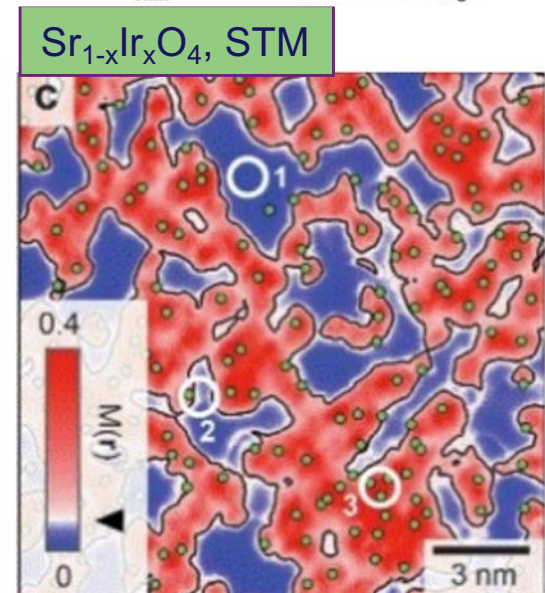
Post, ... KD, EC, ... *et al.*,
Nature Physics (2018)



Lupi *et al.*,
Nature Commun. **1**, 105 (2010)



Battisti *et al.*,
Nature Physics **13**, 21 (2016)

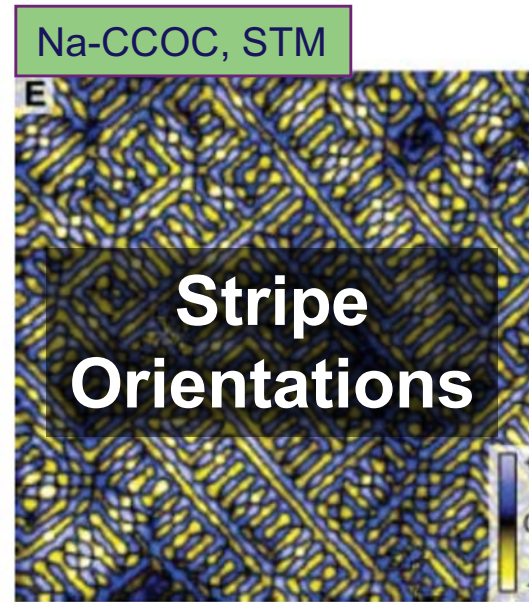


Universal Origin of Patterns?

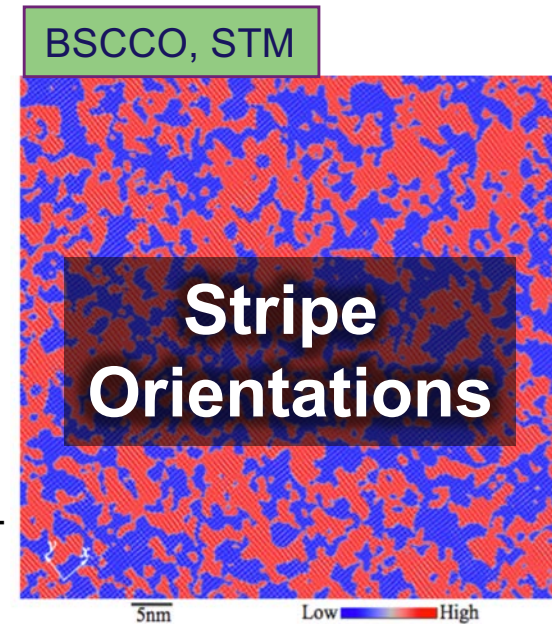
Qazilbash *et al.*,
Science **318**, 1750 (2007)



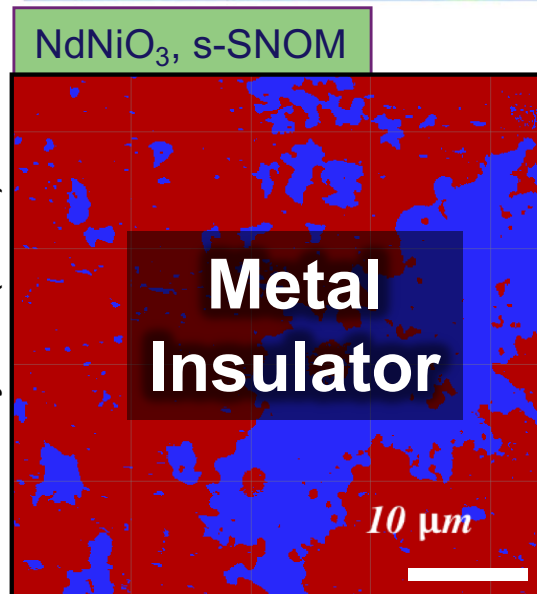
Kohsaka *et al.*,
Science **315**, 1380 (2007)



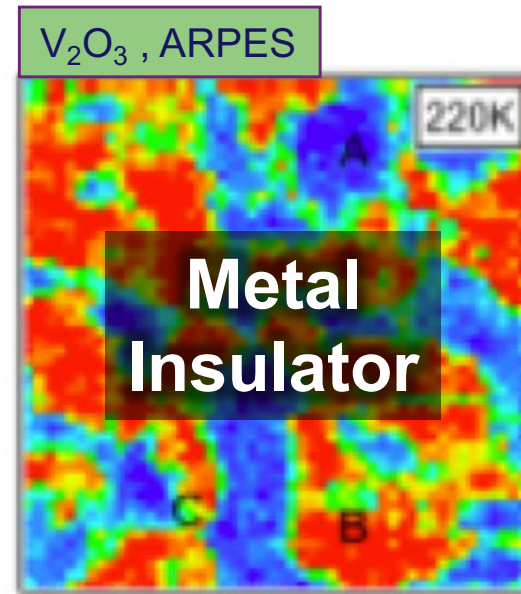
Main, Hoffman, *et al.*,
unpublished



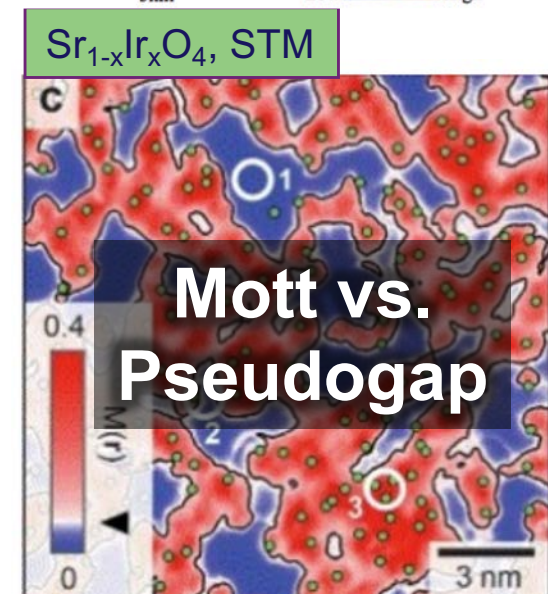
Post, ... KD, EC, ... *et al.*,
Nature Physics (2018)



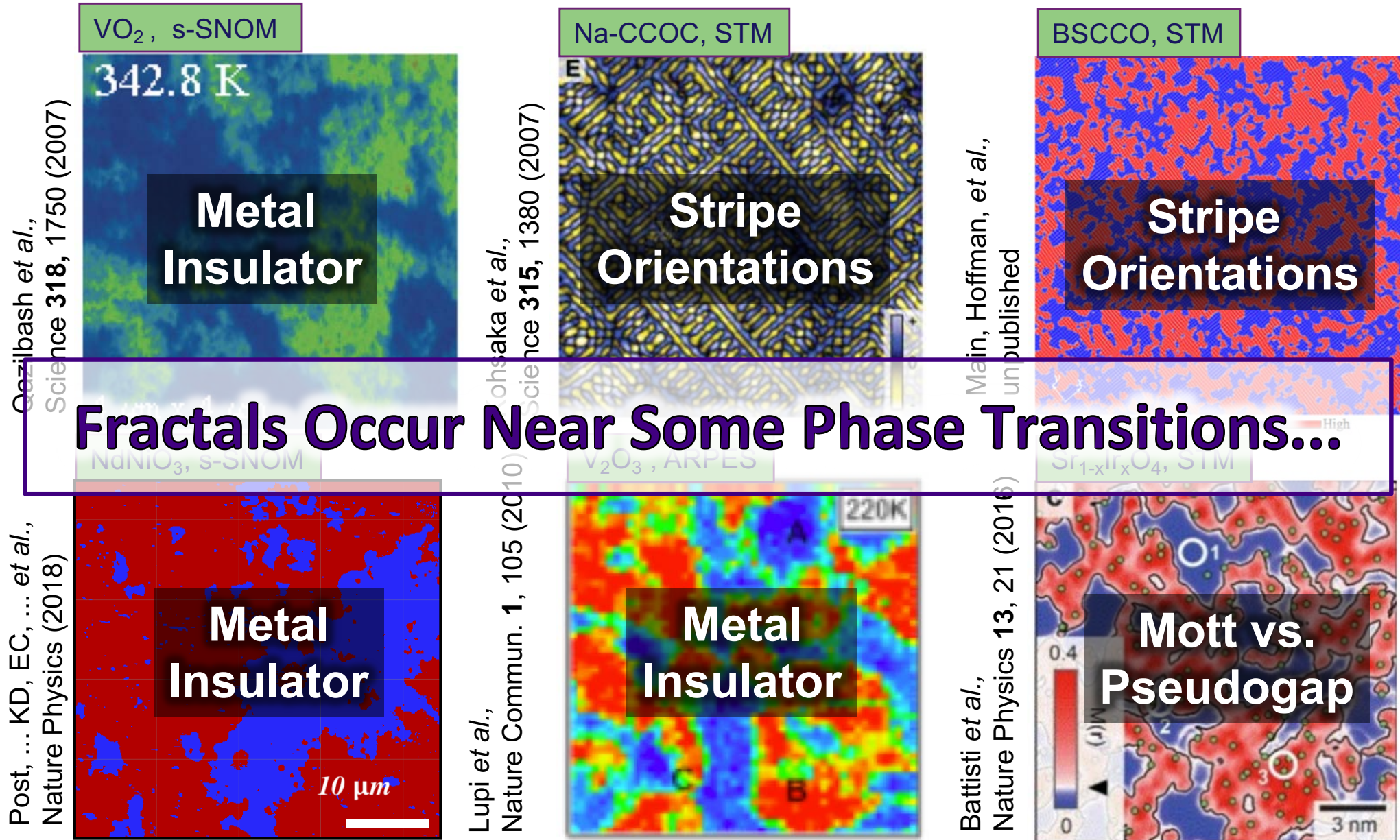
Lupi *et al.*,
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Universal Origin of Patterns?

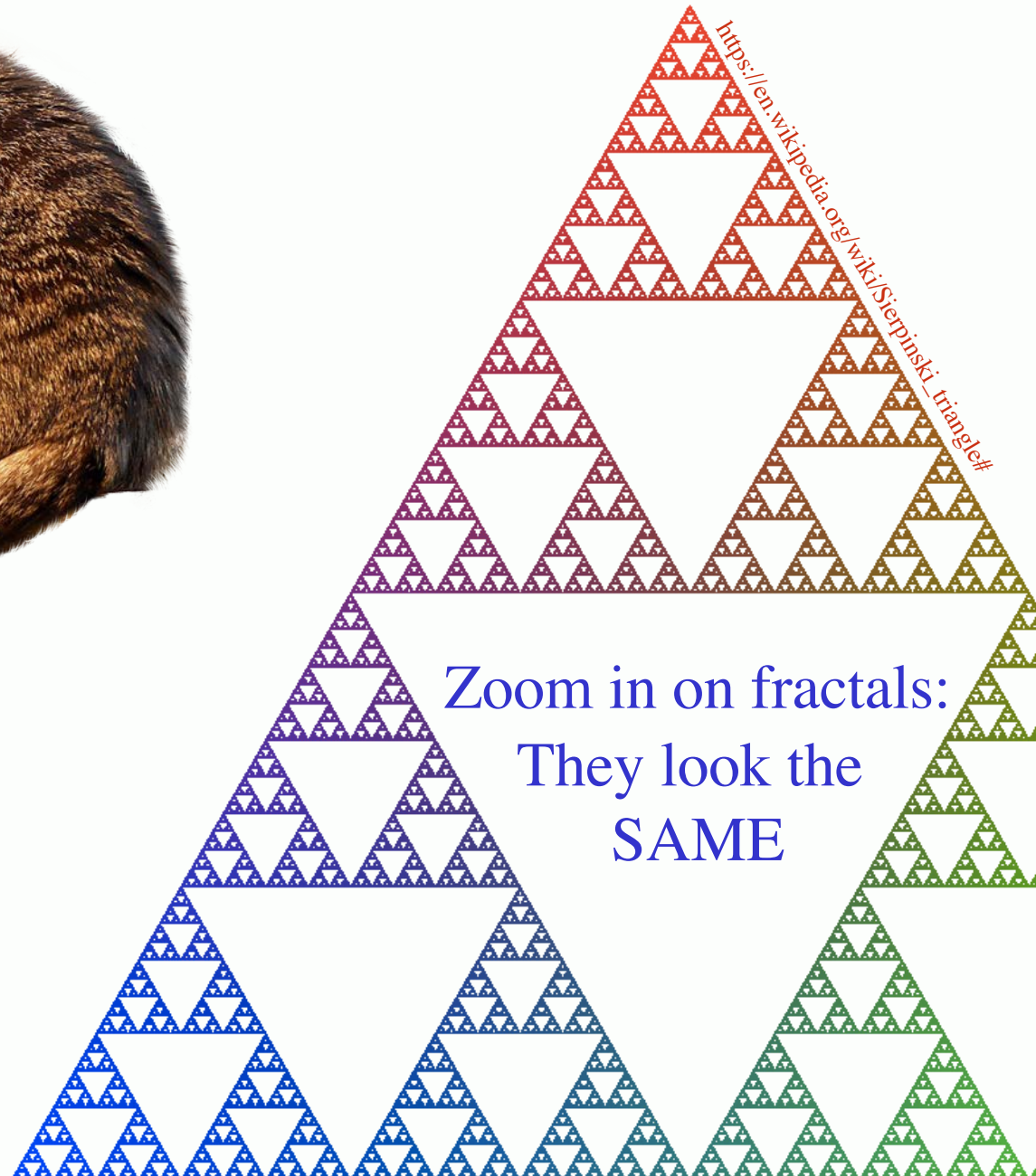


Fractals and “Scale-Invariance”



Zoom in on most objects:
They look quite different

<https://pixabay.com/photos/cat-free-cat-animal-red-tomcat-2973097/>
<https://pixabay.com/photos/cat-fur-cat-mackerel-red-tiger-cat-2694745/>



Zoom in on fractals:
They look the
SAME

What Happens at the *Critical Point* of a Continuous Phase Transition?



Fluctuations at all Length Scales



No Characteristic Length Scale



Fractals!

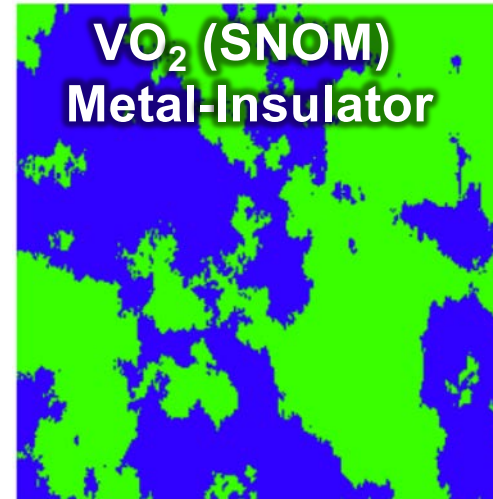
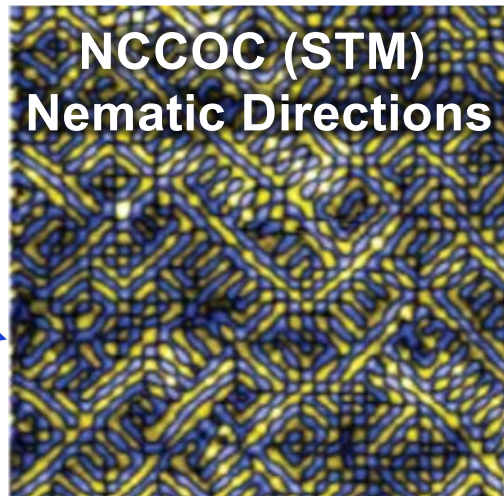
(Universal Power Law Behavior)

***All* mixtures share universal features at their critical point.**

How do we know whether a surface probe measures bulk physics?

Answer: By extracting the fractal dimensions and other critical exponents from the images

Phillabaum, EC, *et al.*,
Nature Commun.,
2012



Liu, EC, *et al.*,
PRL 2016

*These fractals
fills space*



*These fractals
are confined
to a surface*



Critical?

→ If so, Critical Exponents are Encoded in this Pattern

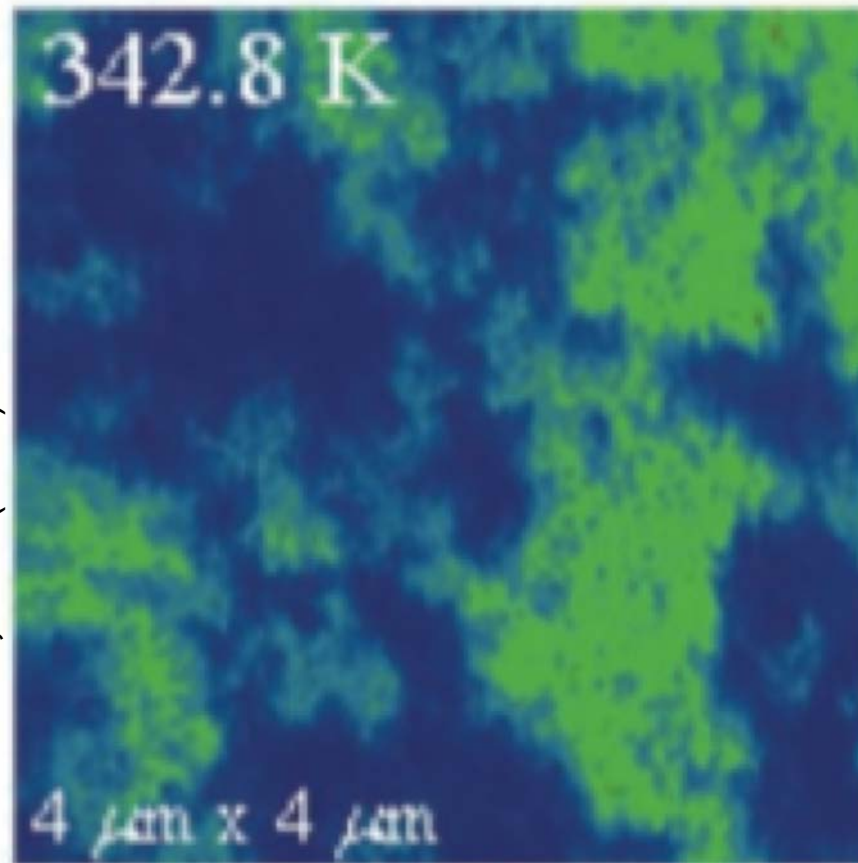
Hull Fractal
Dimension

$$d_h$$

Volume
Fractal
Dimension

$$d_v$$

Qazilbash et al.,
Science **318**, 1750 (2007)



of Clusters
of Each Size

$$\tau$$

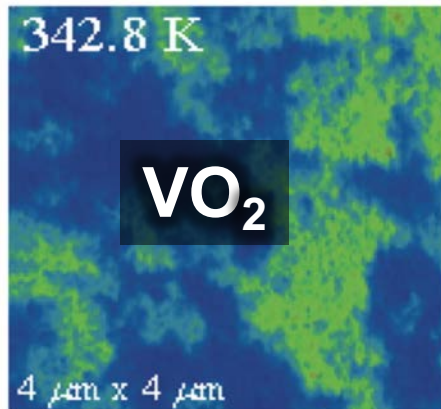
Correlation
Function(s)

$$\eta_{\text{spin}}$$

$$\eta_{\text{cluster}}$$

Universality of Complexity in Disordered Quantum Materials

Qazilbash *et al.*,
Science (2007)

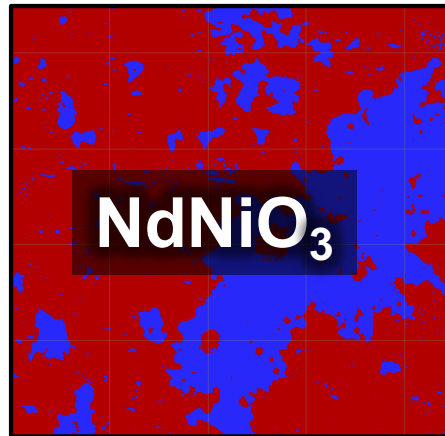


2-Phase + Disorder =
Random Field Ising Model

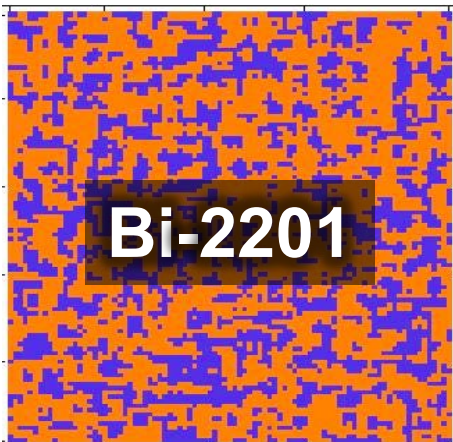
Implications:

- Fractal Clusters
- Glassiness/Aging
- Hysteresis
- Non-Repeatability

Post *et al.*,
Nat. Physics (to appear)



Phillabaum, EC, Dahmen
Nat. Commun. (2012)



VO₂: SL, ... EC, ... Basov, PRL **116**, 036401 (2016)

NdNiO₃: Post, ... YW, EC ... Basov, Nature Physics **14**, 1056 (2018)
Li, ...FS, EC, ... Comin, Nature Commun. **10**, 4568 (2019)

Cuprates: BP, EC, ... Nature Commun. **3**, 915 (2012)

Cluster Methods → Critical Exponents

Advantages

- Extract from Surface Experimental Data:
 - Symmetry of Order Parameter
 - Dimension of Phenomenon (surface or bulk)
 - Type of Disorder
 - Discern Interactions vs. Disorder
- Clear Interpretation via Criticality Theory & RG

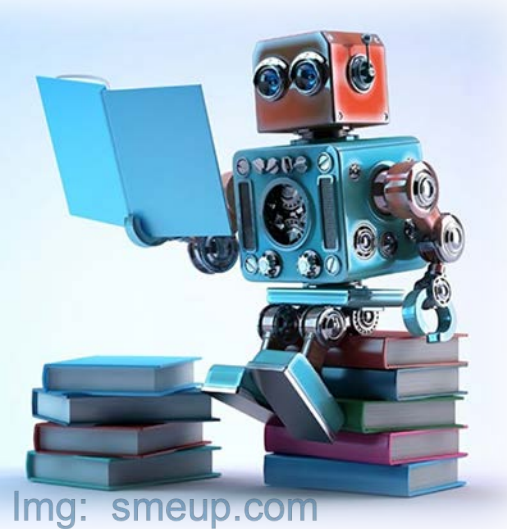
Disadvantages

- Needs 200x200 pixels
- Requires expertise and time

Can ML
Do Better?



Machine Learning in a Nutshell



A computer program exhibits Machine Learning if:

Its ability to perform a Task
Increases with Experience
As determined by some Performance Metric

Program accumulates iterative moderations (Learns)

When presented with multiple instances of input (Experience)

So as to improve (increase Performance Metric)

... Without the modifications being explicitly programmed.

Can ML Identify Which Model Produced Which Critical Spin Configurations?

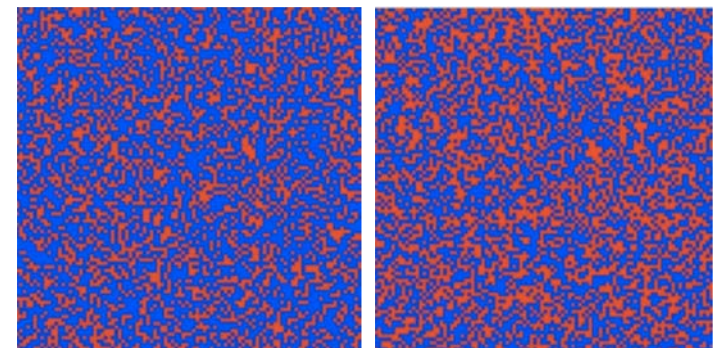
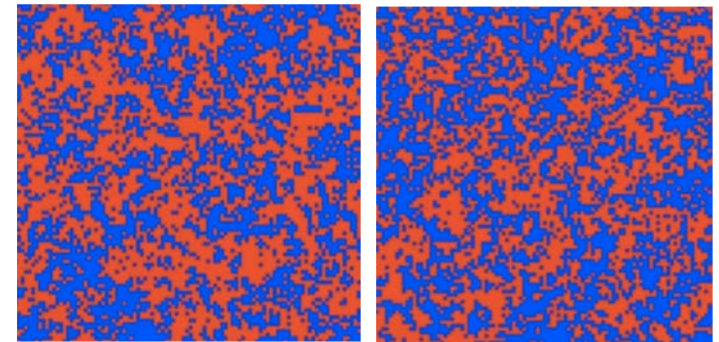
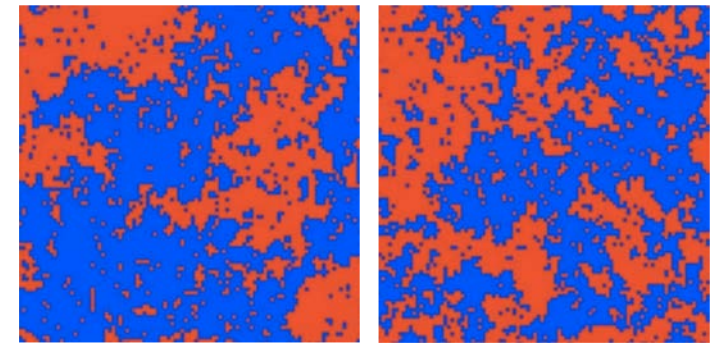
Ultimate Goal: Classify Scanning Probe Data. First Step: Classify Simulation Results

2D and 3D Clean Ising Model

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

Two Dimensional
 $L^2=100^2$

Three Dimensional
 $L^3=100^3$



Uncorrelated Percolation Model

Sites occupied with probability p

$L^2=100^2$

Can ML Identify Which Model Produced Which Critical Spin Configurations?

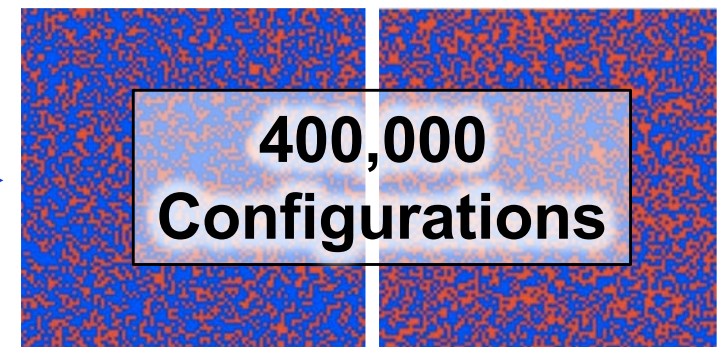
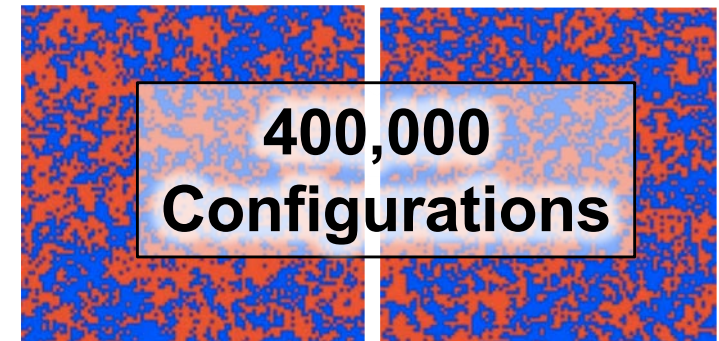
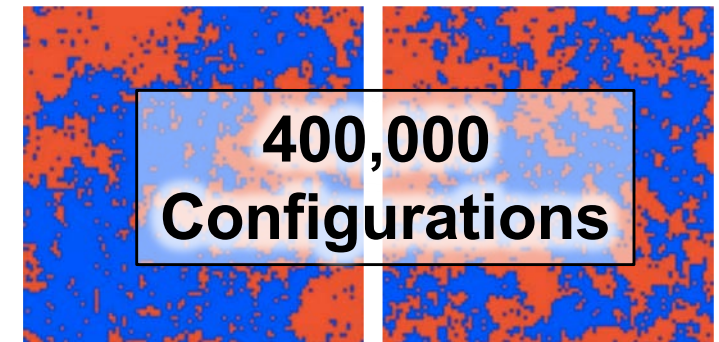
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$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

Two Dimensional
 $L^2=100^2$

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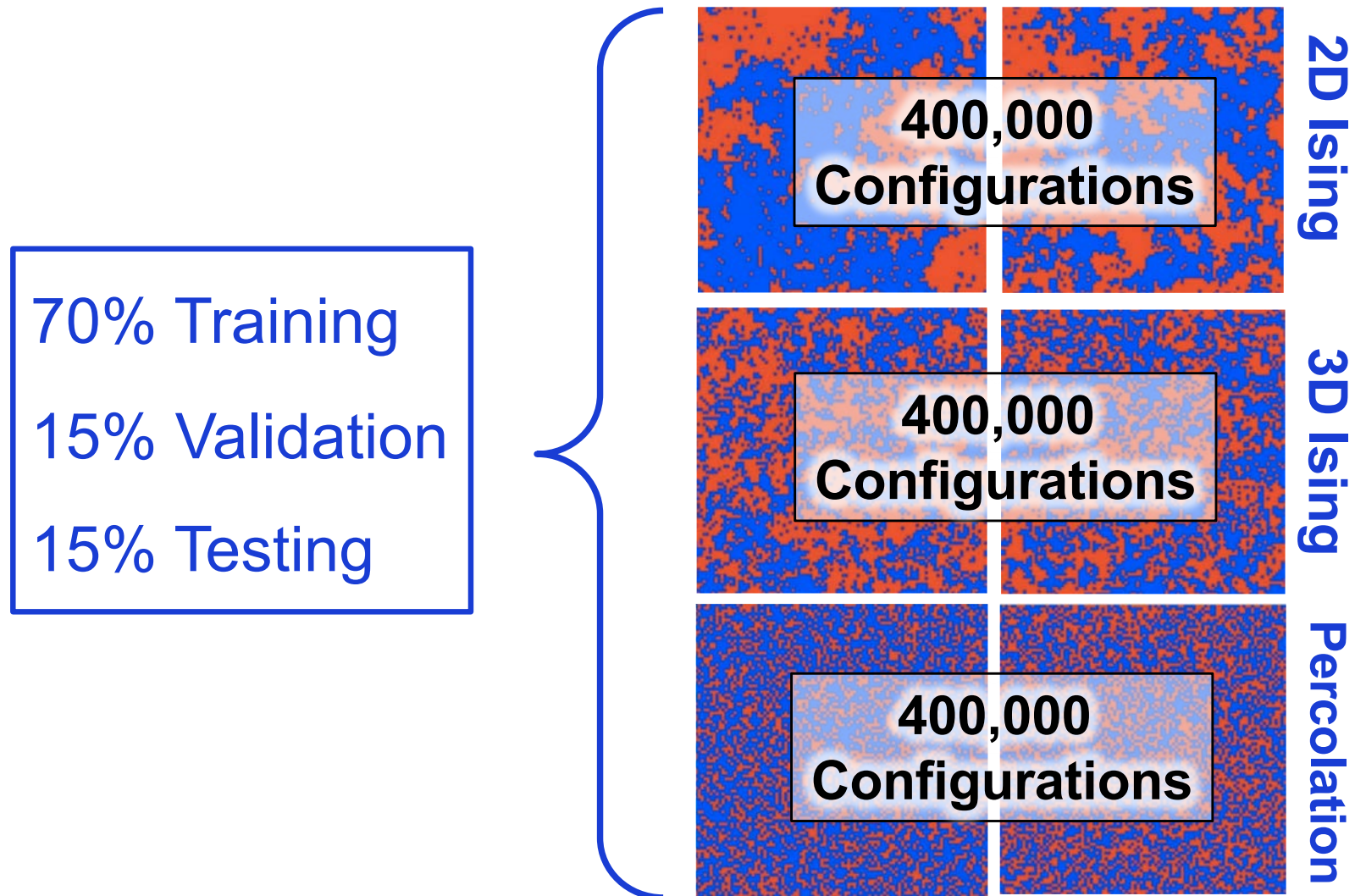


Uncorrelated Percolation Model

Sites occupied with probability p $\xrightarrow{L^2=100^2}$

Can ML Identify Which Model Produced Which Critical Spin Configurations?

Ultimate Goal: Classify Scanning Probe Data. First Step: Classify Simulation Results





The Whole Process in a Nutshell

Monte Carlo Simulations
Generate Images

2D Ising

**Training
Configurations**

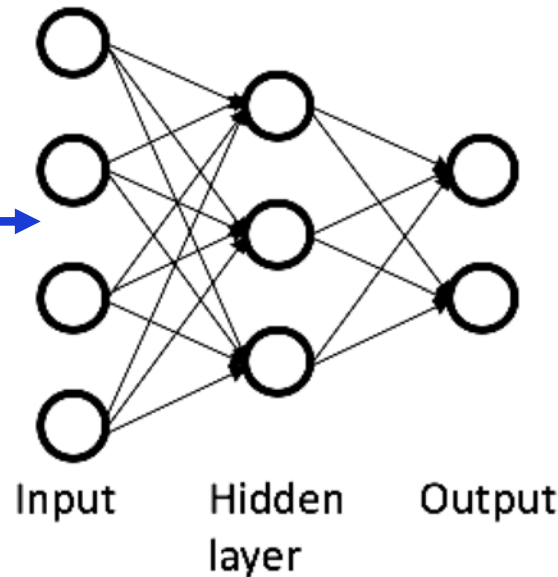
3D Ising

**Training
Configurations**

Percolation

**Training
Configurations**

Machine Learning Algorithm
Learns to Classify Images



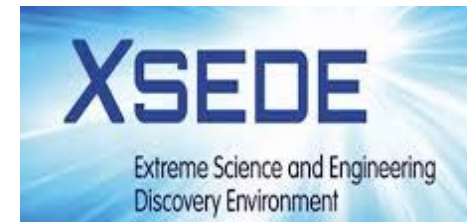
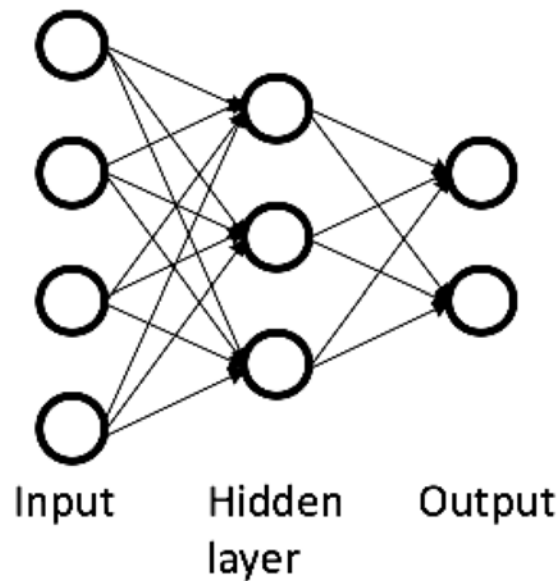
“2D Ising”
“3D Ising”
“Percolation”

Use Validation Set to
Determine “hyperparameters”:

- Number of hidden layers (1)
- Number of hidden neurons (200)



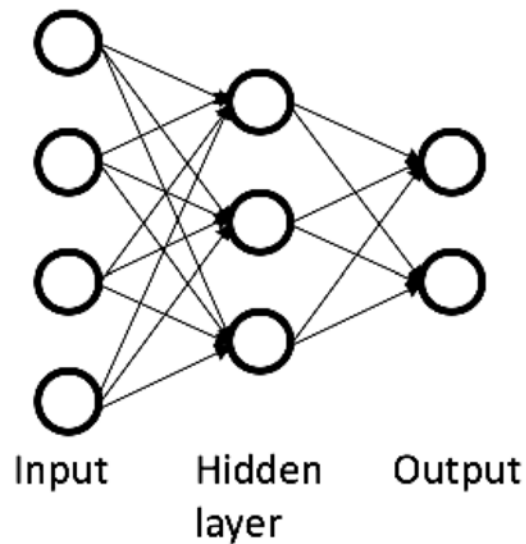
Inside the Nutshell



MATLAB Neural Network Toolbox on XSEDE

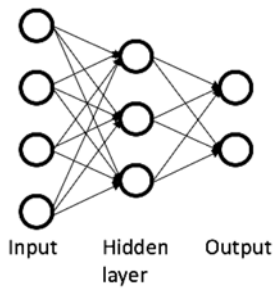
- Supervised Learning
- Scaled Conjugate Gradient Algorithm
- Single hidden layer (50-250 neurons)

Results From Validation Sets



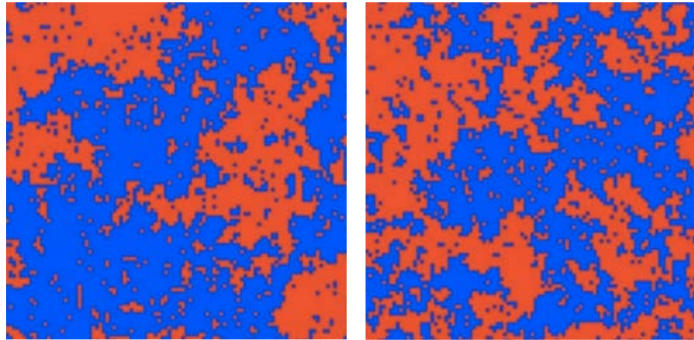
Hidden Neurons	% Accuracy
50	94.93
75	95.53
100	95.95
125	96.48
150	96.68
200	97.00
250	96.72

Therefore, we choose 200 Hidden Neurons

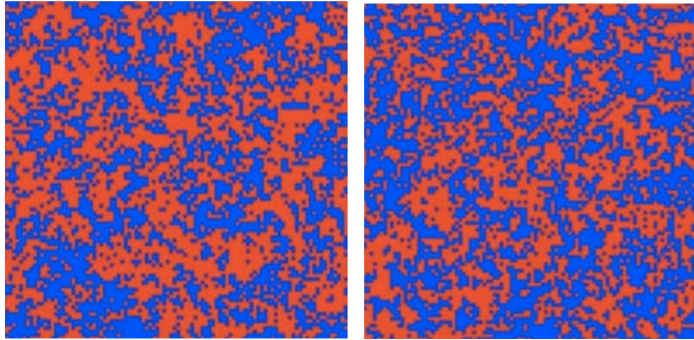


Results of the Trained ML Model With 200 Neurons

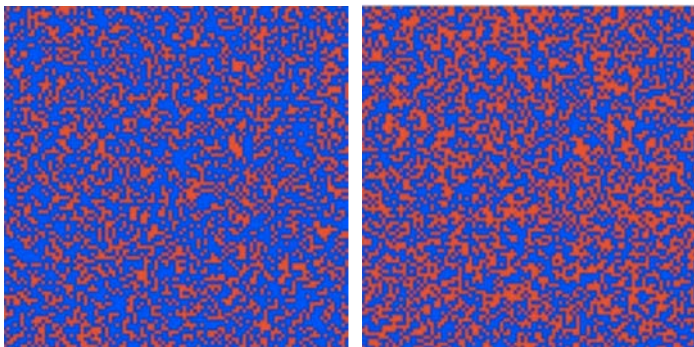
2D Ising



3D Ising



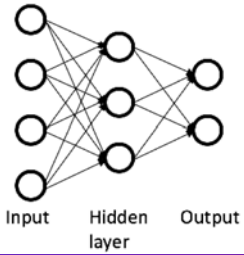
Percolation



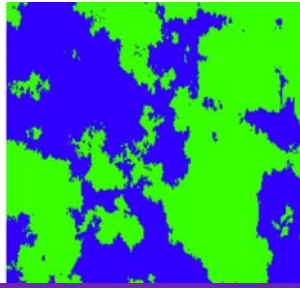
		Neural network output		
		perc	I-2D	I-3D
Input	perc	98.05%	0.01%	1.94%
	I-2D	0.03%	98.30%	1.67%
	I-3D	1.82%	2.96%	95.22%

- ML Distinguishes Ising from Percolation Very Well
- Harder to distinguish 2D from 3D

CURRENT WORK (with Sayan Basak)
Convolutional Nets can get 99.9%



Summary and Future



Critical Exponent Method:

- Clear Interpretation
- Needs 200x200 pixels
- Requires expertise and time

Nature Commun. 10, 4568 (2019)

Nat. Phys. 14, 1056 (2018)

Phys. Rev. Lett. 116, 036401 (2016)

Nature Commun. 3, 915 (2012)

ArXiv:1803.08485

Machine Learning Method:

- “Black box”
- Works on smaller FOV
- Scalable, Shareable

Phys. Rev. Mat. 3, 033805 (2019)

CURRENT WORK: - Train to distinguish Random Field Ising Models
 - Apply to real datasets!

FUTURE WORK: - Extend beyond Criticality and beyond Ising