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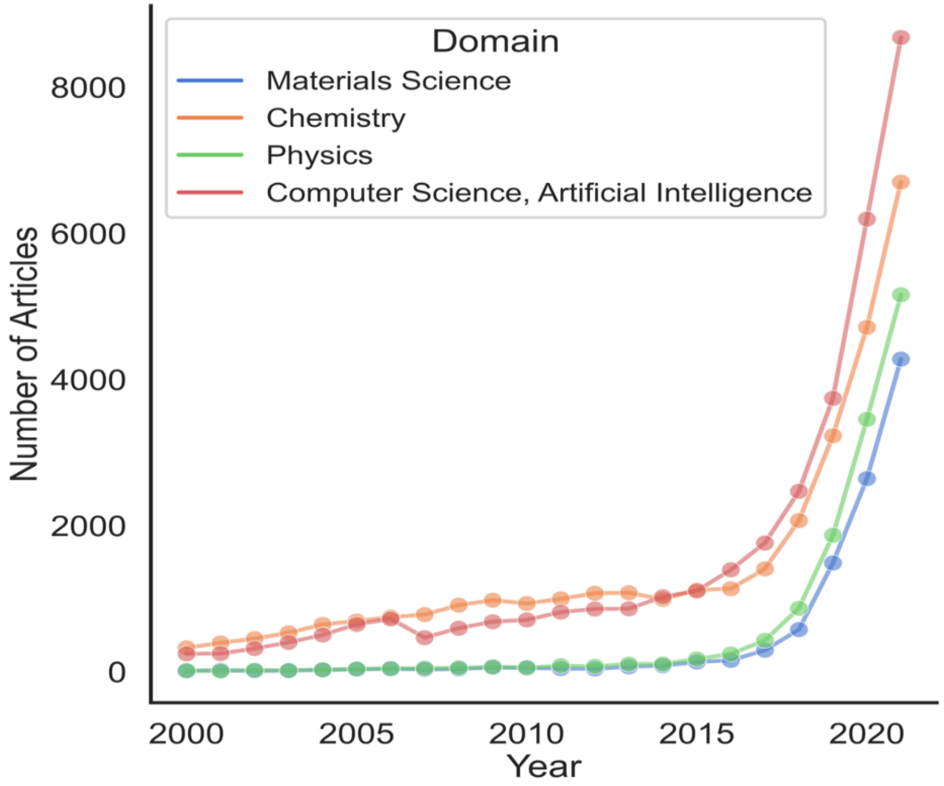
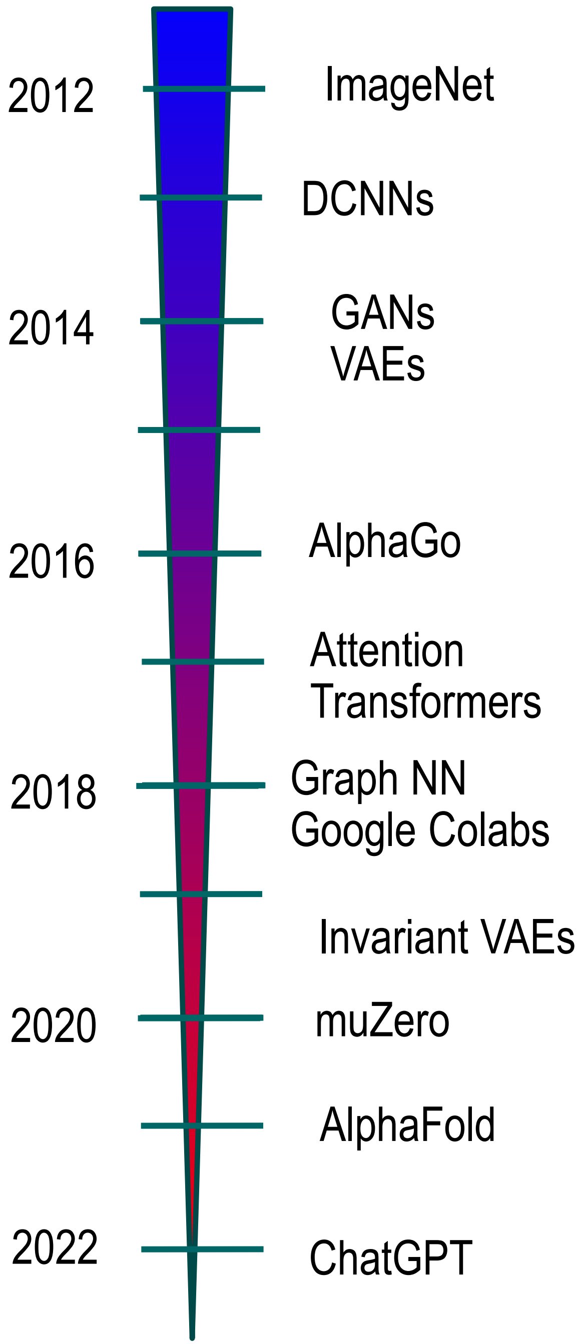
Neural Networks: Shallow and Deep

Sergei V. Kalinin

Why machine learning in imaging?

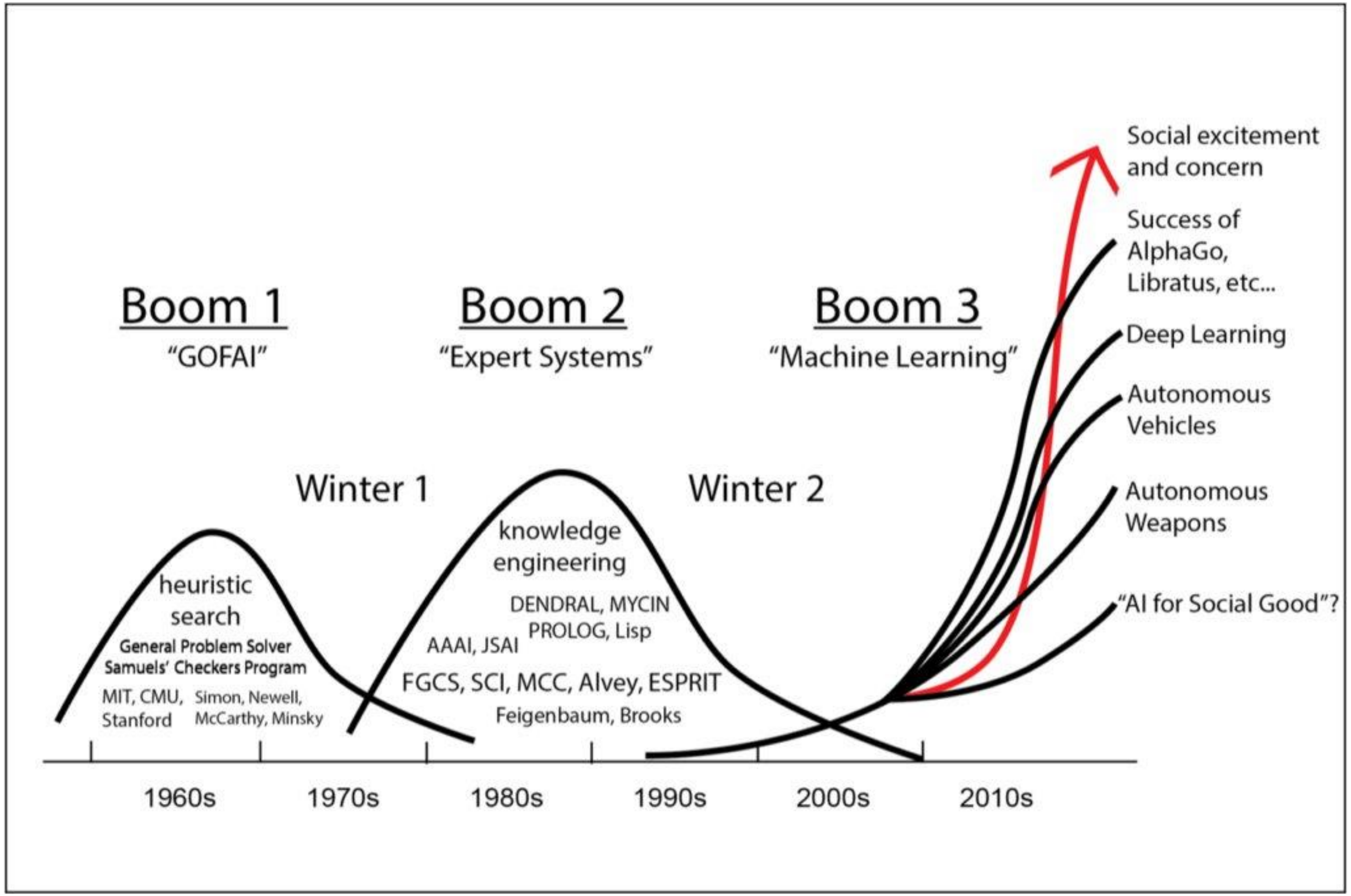


Analysis by B. Blaiszik, Argonne



- Last decade has experienced an explosive growth of machine learning and artificial intelligence applications
- These developments have spanned areas from computer vision to medicine to autonomous systems and games
- However, the progress and impact as applied to experimental physical sciences has been minimal….

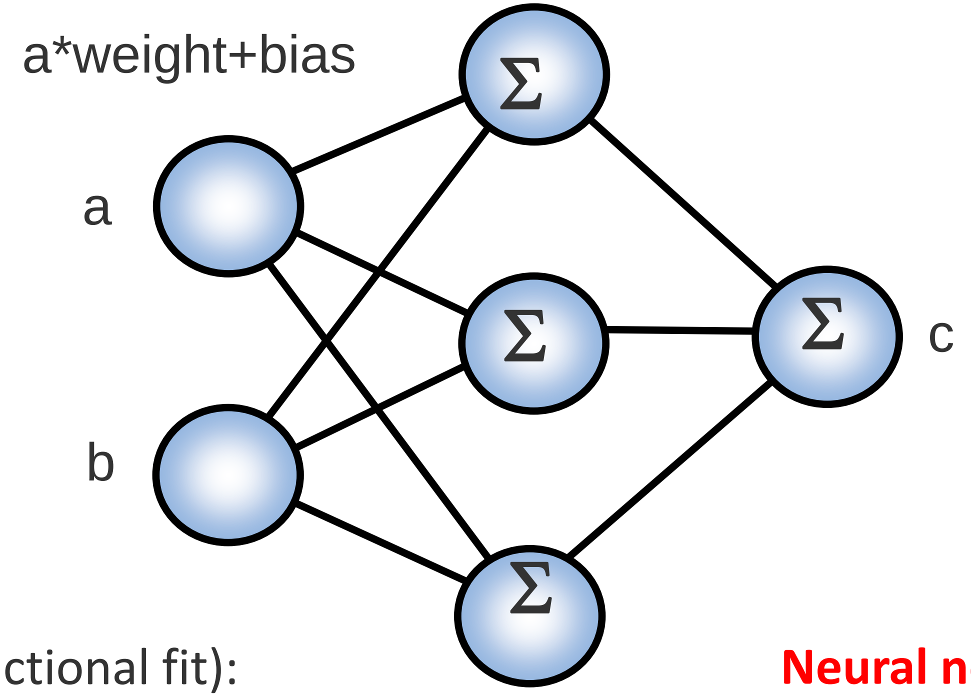
Zooming out on history



https://jaylatta.net/history-of-ai-from-winter-to-winter/

Enter the neural network

- An **artificial neural network (ANN)**, is a mathematical model based on biological neurons.
- Interconnected group of artificial neurons and processes information using a connectionist approach
- Changes its structure in response to information flow during the learning phase.
- NN's can be used as **universal interpolators** which relate large families of inputs to outputs



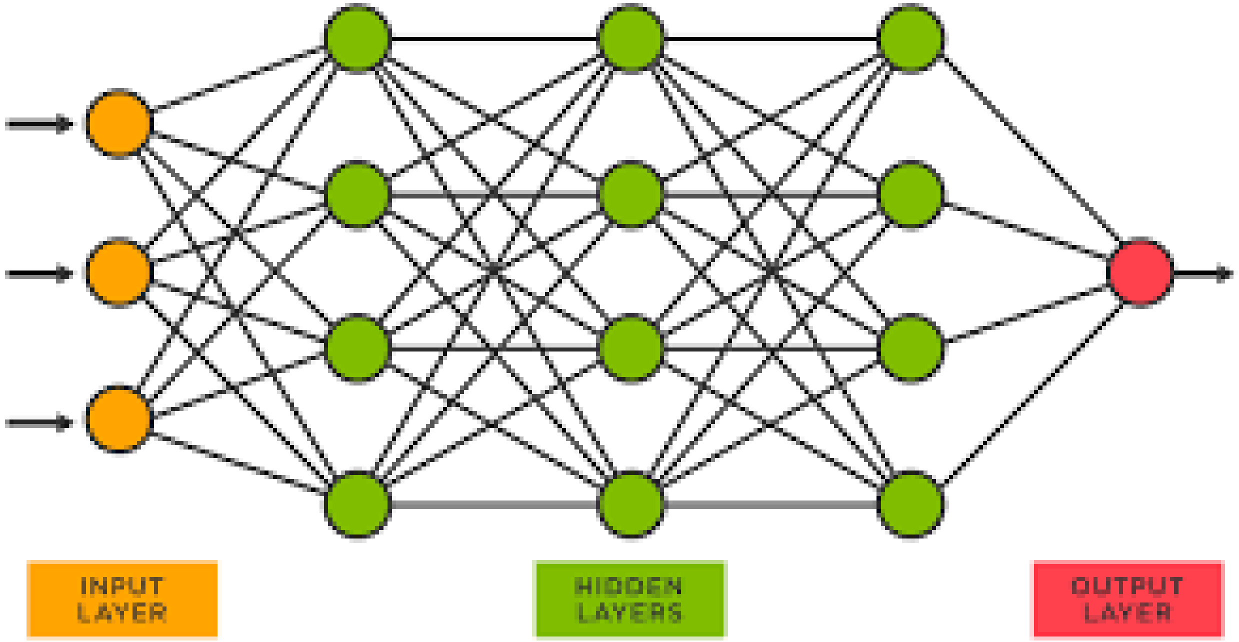
Classical approach (functional fit):

- Need model knowledge
- Fit is reasonably slow
- Cannot be implemented in real time
- Ideal for single task if physics is known

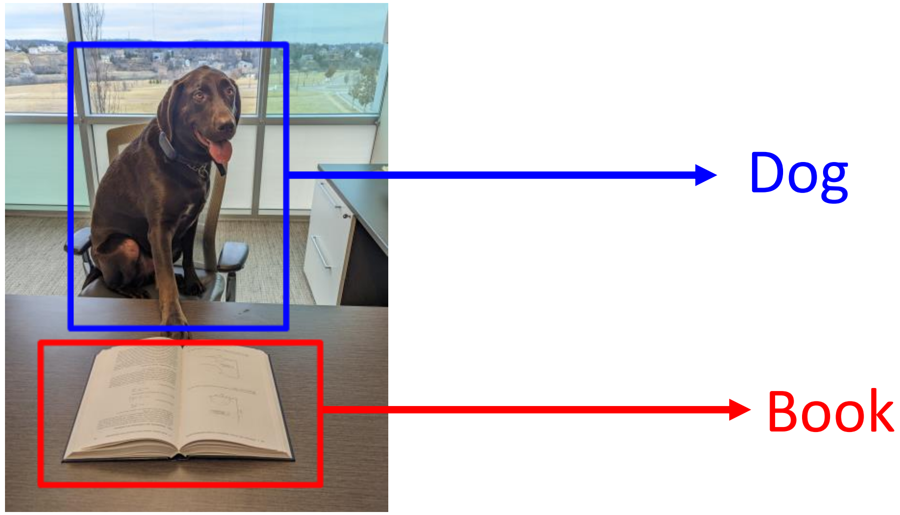
Neural network approach

- Training is time consuming
- Recognition is very fast
- Can be implemented in real time
- Ideal for multiple similar tasks

What is machine learning?



- Supervised machine learning
- Unsupervised machine learning
- Semi-supervised machine learning
- Reinforcement learning



Drivers beyond ML development

- **Before 2000:** It's all about IT (dotcoms, Amazon, etc)
- **2000 - 2010:** It's all about collecting and searching data (Facebook, Google, Uber, etc.)
- **2010 – 2020:** What do we learn from data (correlative era)
- **2020 – now:** Physics is the new data

arXiv:2204.05095

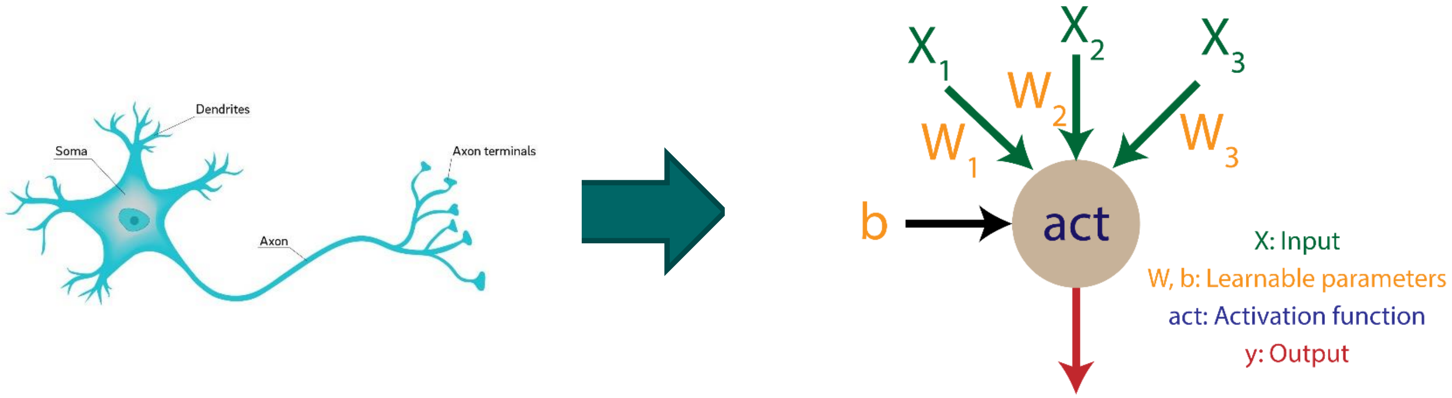
- Classical machine learning is underpinned by the existence of the large static data sets – from MNIST to emerging medical, bio, faces, etc.
- Real world problems are associated with the large distribution shifts, often small data sets, and presence of uncontrollable exogenous factors
- Also, real world problems are often active learning: we interrogate the data generation process and provide feedback, not deal with static data sets
- However, we often have extensive prior knowledge of past data, physical laws generalizing them, and strong set of inferential biases

arXiv:2005.01557

Microscopy is an ideal playground for active learning!

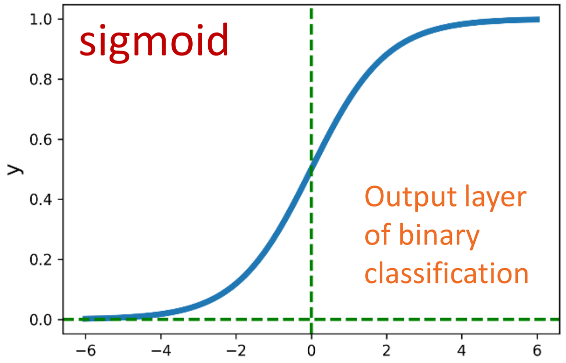
Elementary neuron and activation function

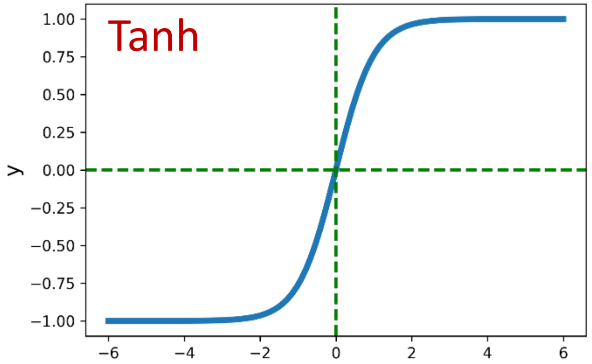
- Artificial neuron is weakly inspired from the biological neuron
- Biological neuron receives its inputs from dendrites, decides whether to fire, and communicates its output *via*., axon terminals

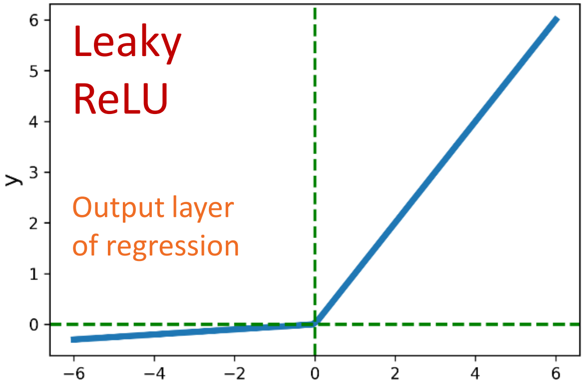


$$y = act(W_1X_1 + W_2X_2 + W_3X_3 + b)$$

- Activation functions introduce non-linearity to the neuron's output.
- Without them, the whole neural network can be replaced by a simple linear regression.







- Softmax activation function is another widely used activation function
- Usually, in the last layer of multi-class classification problem

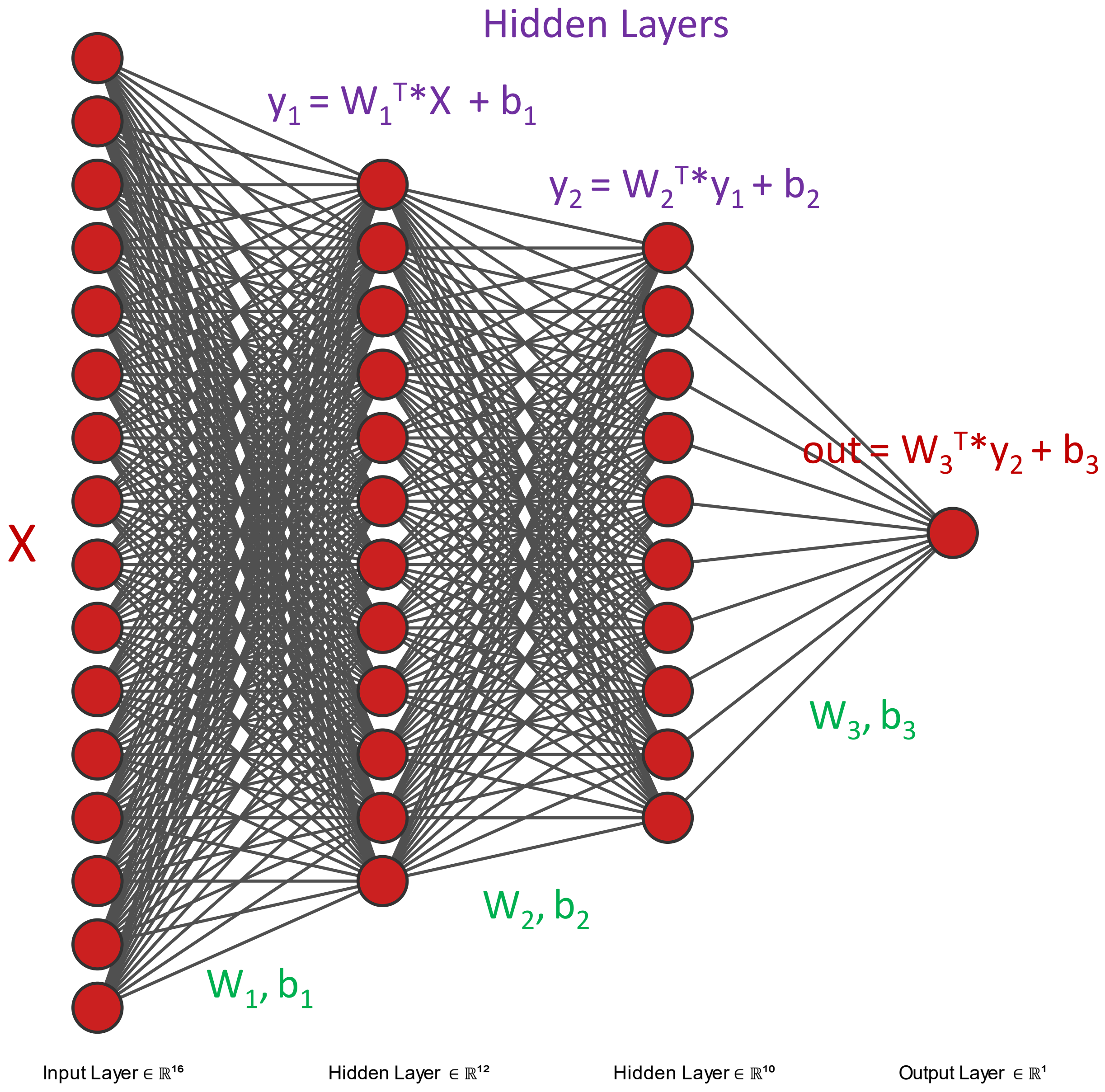
Fully connected (FC) neural network (a collection of neurons)

- Composed of multiple layers of artificial neurons, mirroring the complexity of a human brain.

- Each layer processes inputs received, applies a transformation (weights, biases, activation function), and passes the output to the next layer.

- Training a DNN involves adjusting weights and biases using backpropagation and a chosen optimization algorithm.

- The deep architecture enable the network to learn complex and abstract patterns in data.

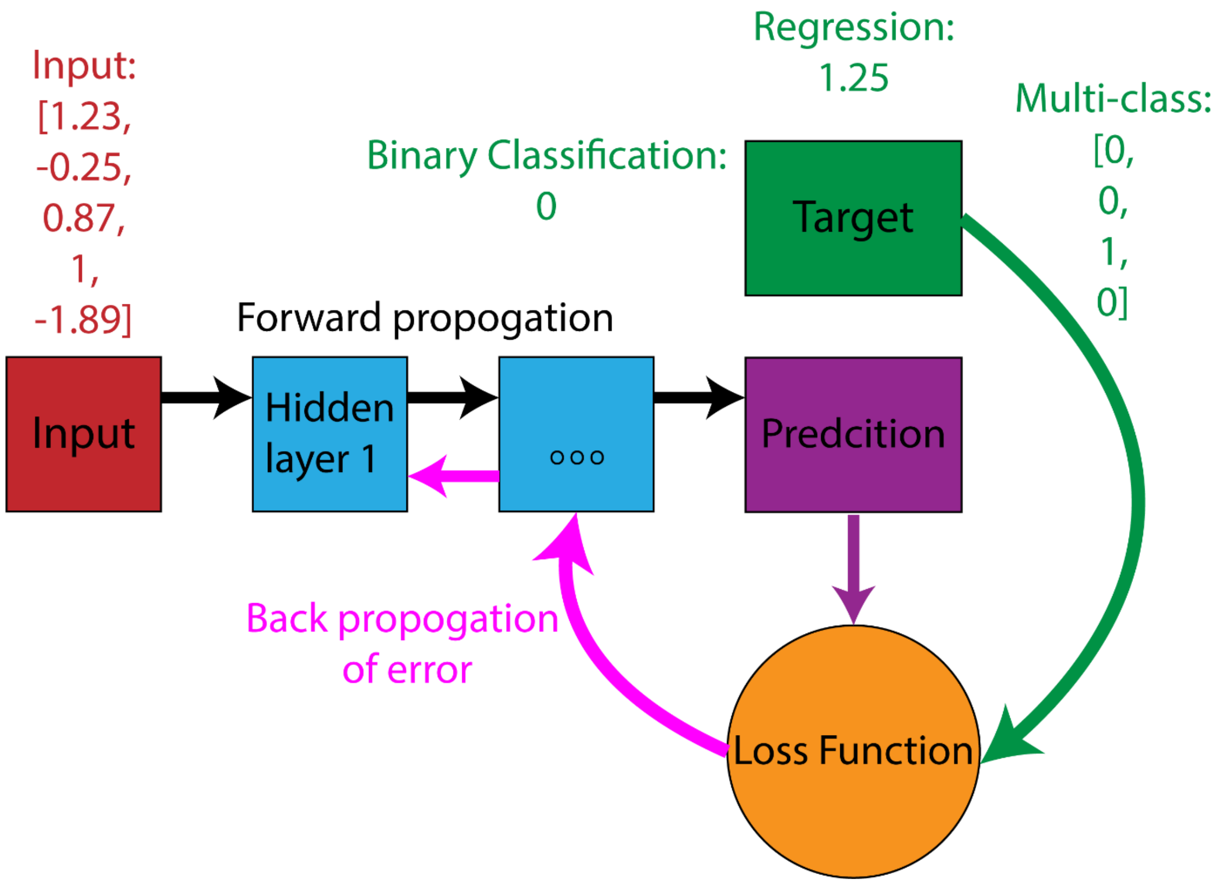


ML tasks

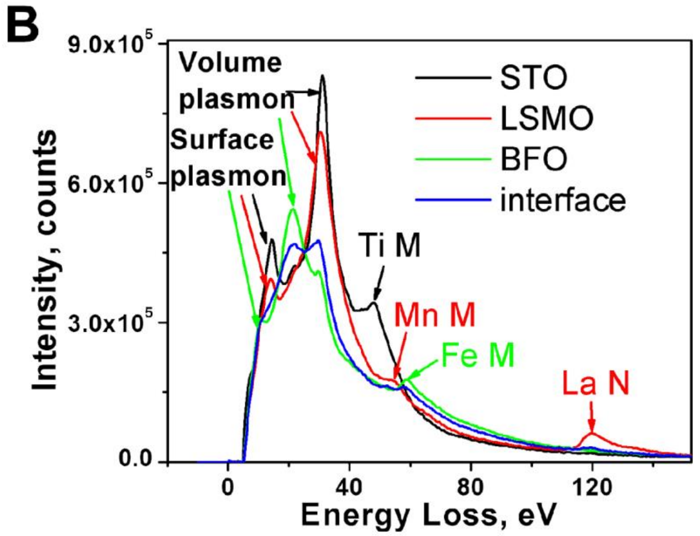
- **Input:**
  - Typical input to a FCNN is a column vector of features that describe a datum.
  - The features are usually independent of each other.
  - Advanced network architectures deal with spatially correlated data (CNN), temporal data (RNN), and graph data(GNN).

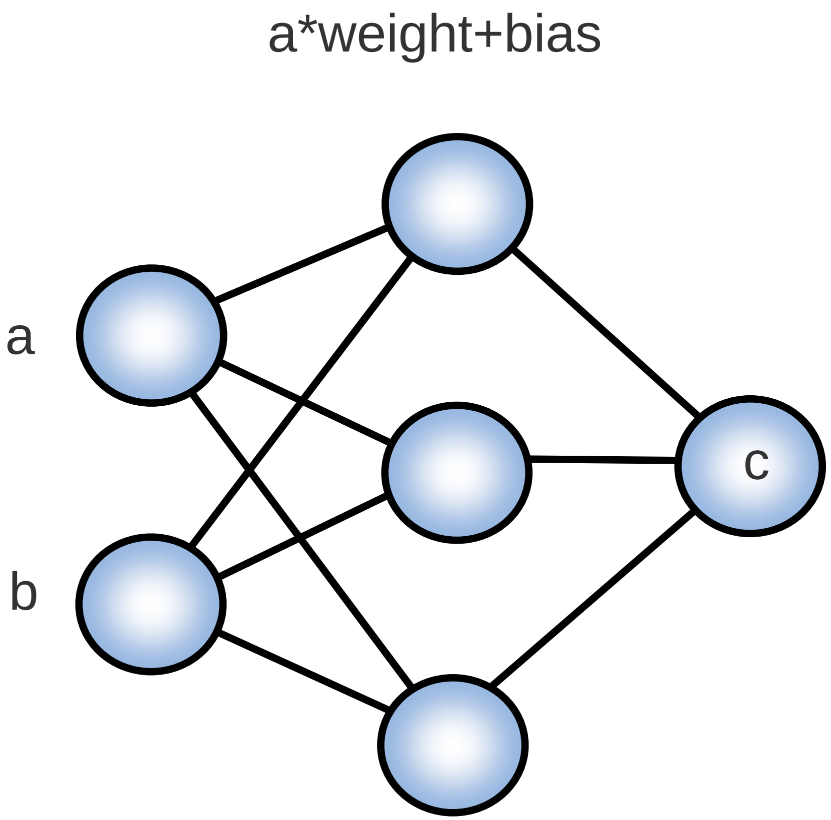
- **Regression**
  - **Target:** Continuously varying quantity
  - **Loss Functions:** Root mean squared error (RMSE), Mean absolute error (MAE)

- **Classification**
  - **Target:** Divided into classes
    - 0 or 1 for a binary class classification
    - One-hot encoded vector for multi-class classification
  - **Loss Functions:** Binary cross entropy loss (BCE) for binary classification and cross-entropy loss (CE) for multi-class classification



Simple example: NN on EELS data



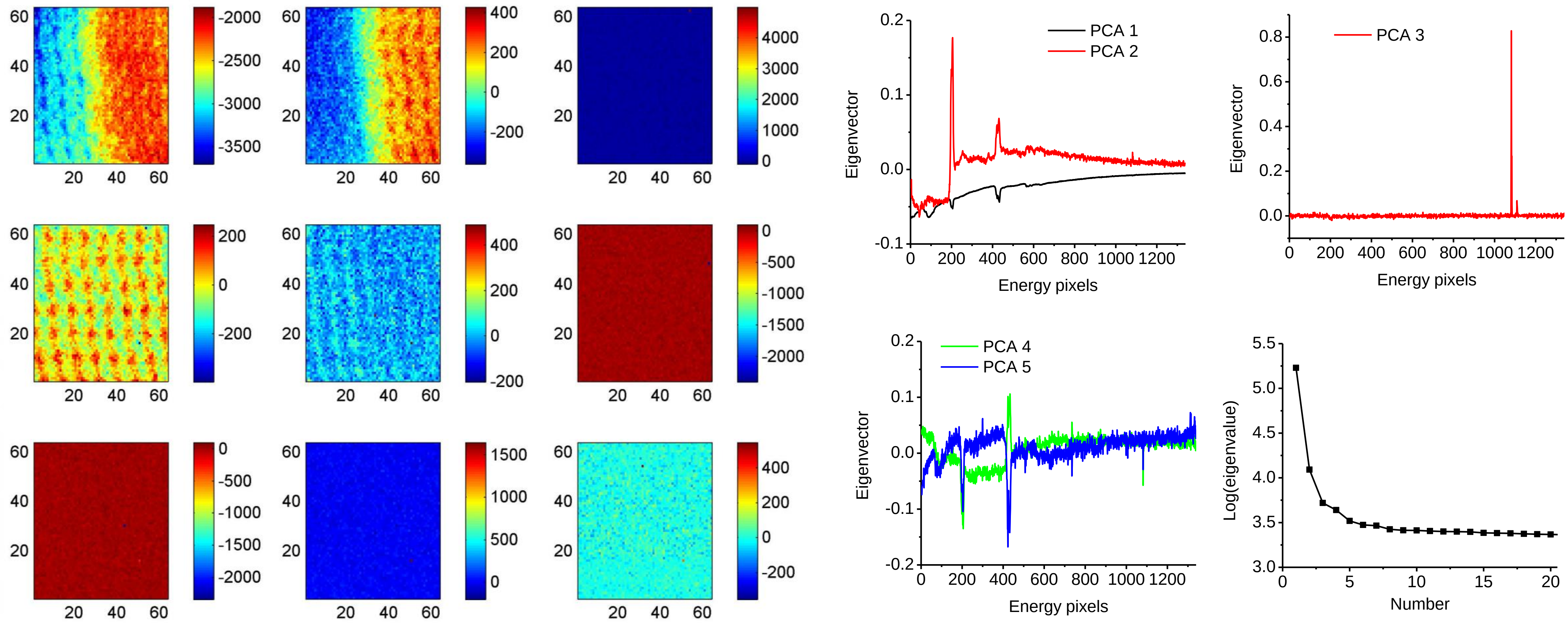


Material:
- STO
- LSMO
- BFO

If we have EELS data set, we can define three types of problems:

- **Physics based analysis:** identify compositions, orbital populations, dielectric function, etc. using known model
- **Unsupervised learning**: discover intrinsic variability in the EELS data set
- **Supervised learning:** identify EELS spectra following some examples

EELS on the $CaTiO_3$-$SrTiO_3$ heterostructure



Data by A. Lupini

- Maps clearly identify components
- The subsequent maps are noise
- Note that maps without structure are dominated by outliers
- Maps show remarkable difference in contrast and symmetry

Shallow NN Analysis

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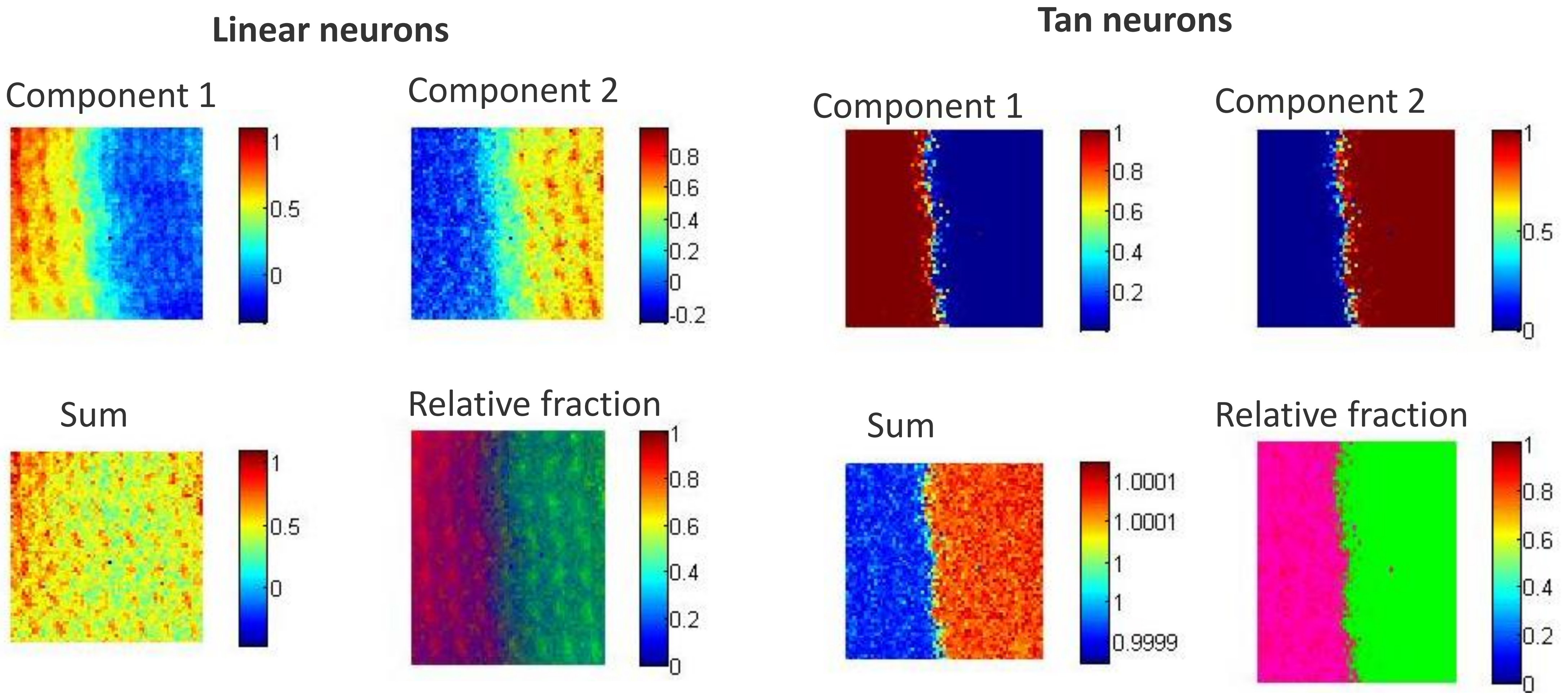
- **Training set:** subset of the image with known composition (or curated label set)
- **Recognition:** full image



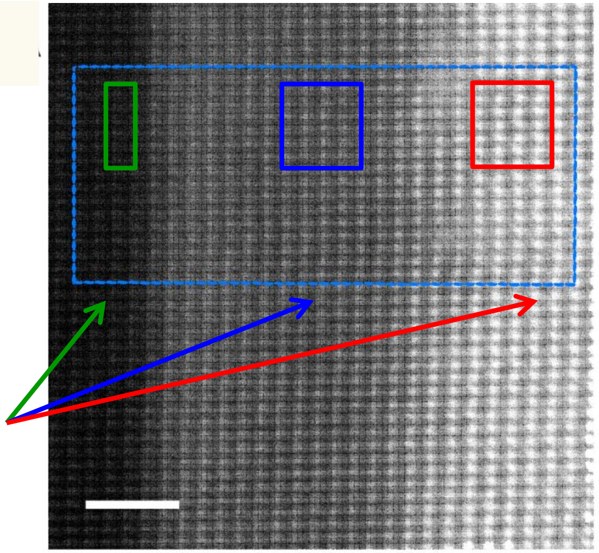
Data A. Lupini, analysis S.V. Kalinin, unpublished (2010)

EELS on LSMO-STO-BFO

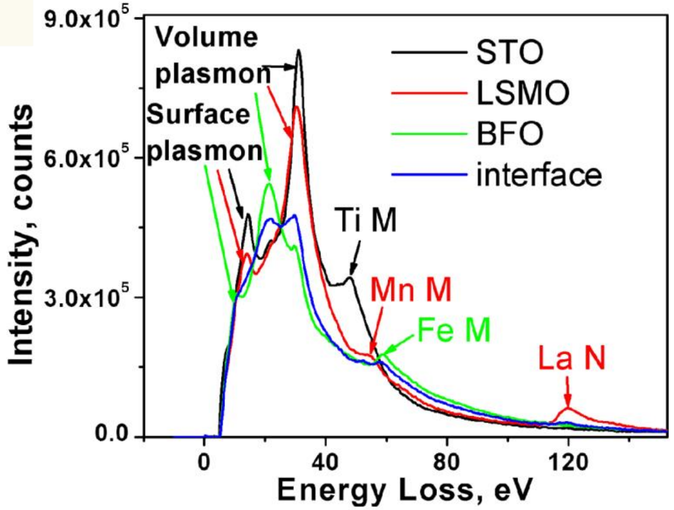
Linear mixing $S(\mathbf{x},\mathbf{R}) = \sum_i a_i(\mathbf{x}) \boxed{w_i(\mathbf{R})}$ +N but $w_i(\mathbf{R})$ are **known**

STEM of STO/LSMO/BFO interface

Standard spectra



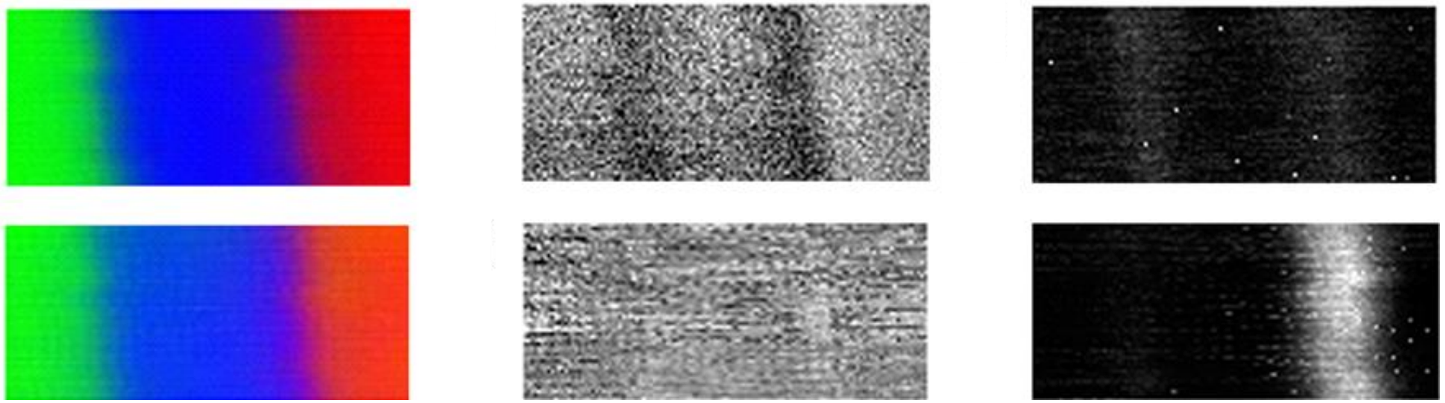
Low-loss EELS spectra of three components



Fit coefficient map **Residuals map** **χ2 map**

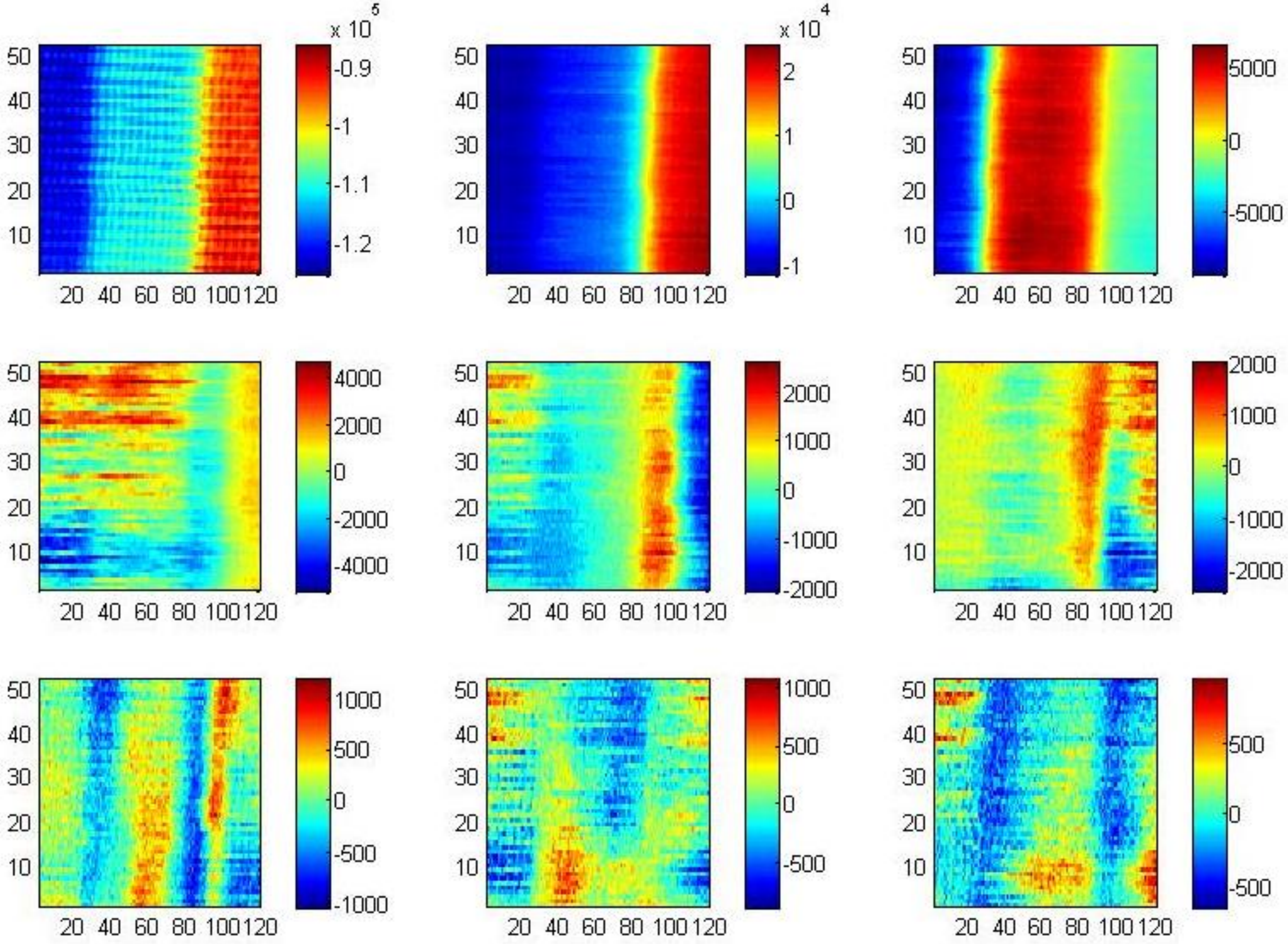
"Chemistry" 35 to 125 eV

"Plasmons" 5 to 35 eV



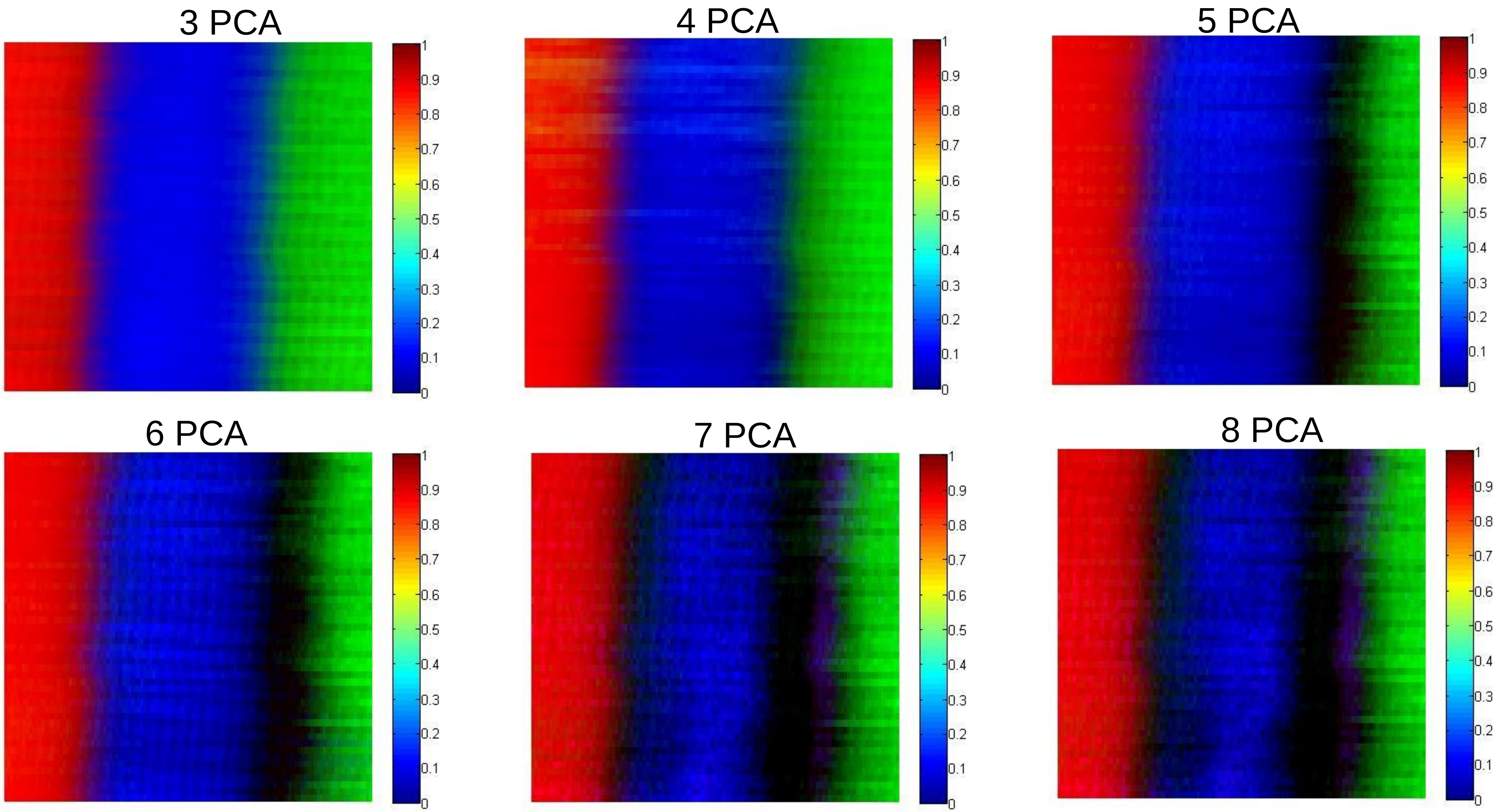
A.Y. Borisevich et al, Phys. Rev. Lett. **105**, 087204 (2010).

PCA Analysis: loadings



DATA FROM A.Y. BORISEVICH ET AL, Phys. Rev. Lett. **105**, 087204 (2010).

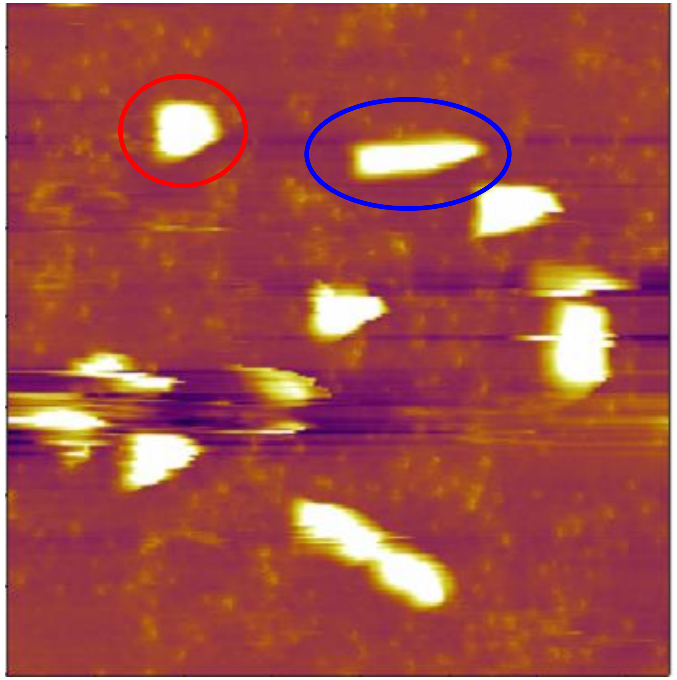
Recognition imaging: STO – LSMO - BFO



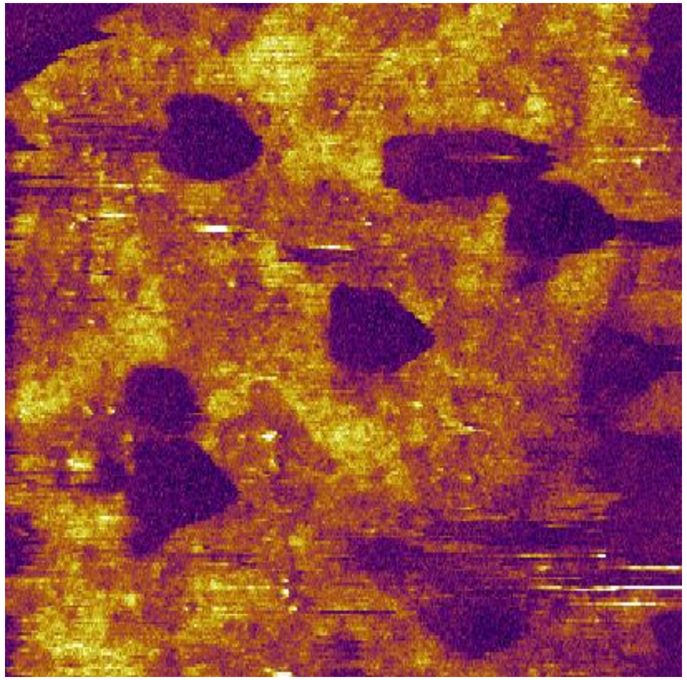
Data A. Borisevich, analysis S.V. Kalinin, unpublished (2010)

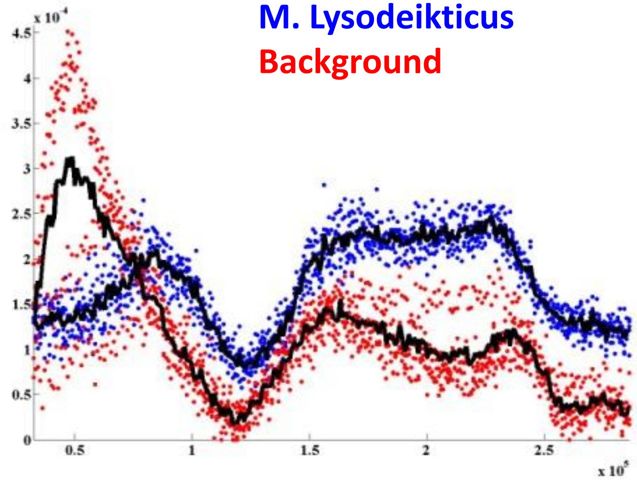
Electromechanical probing of bacteria

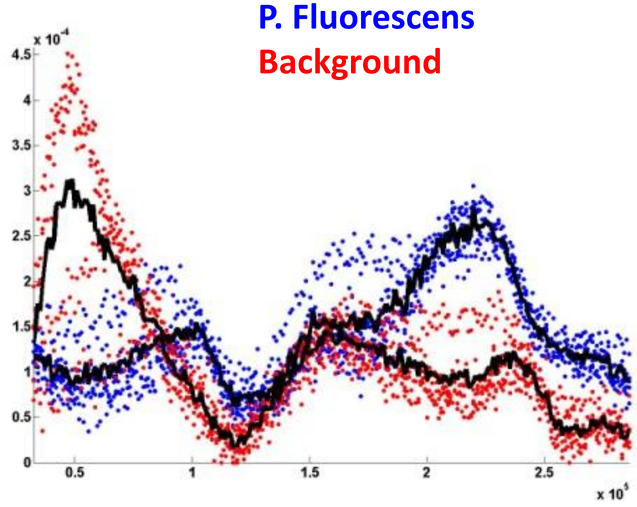
Topography



PFM Amplitude

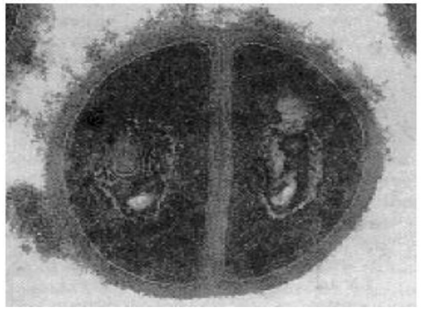






M.P. NIKIFOROV, ET AL
Nanotechnology **20**, 405708 (2009).

M.Lysodeikticus



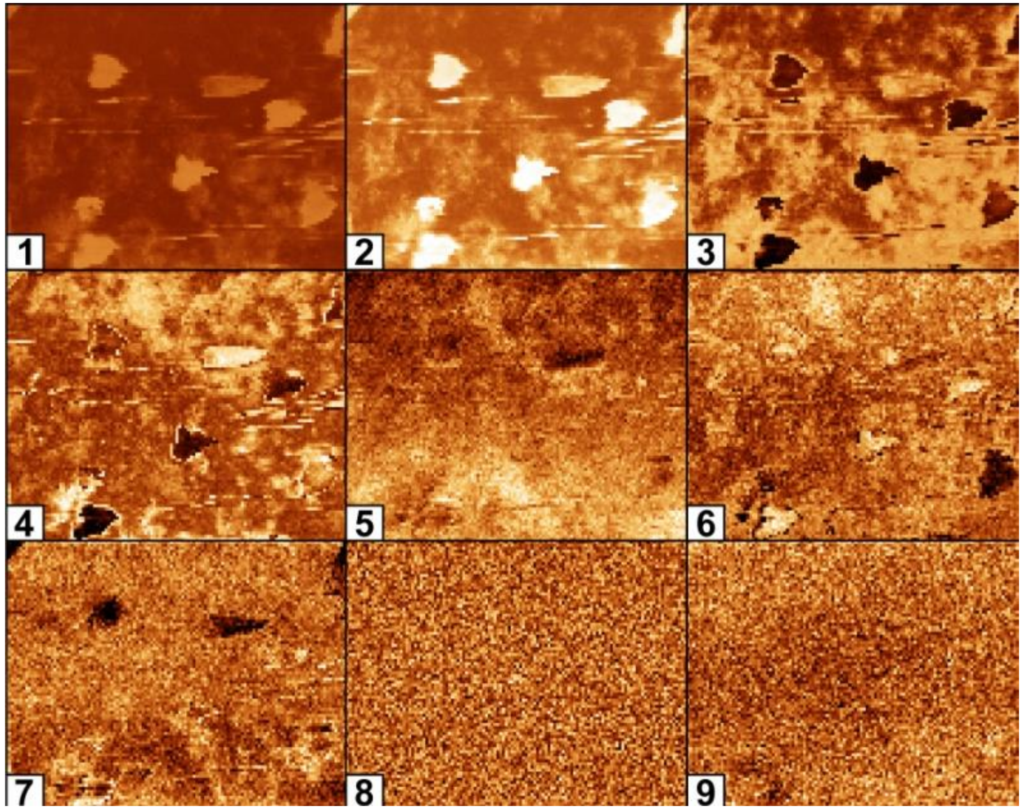
P.Fluorescens

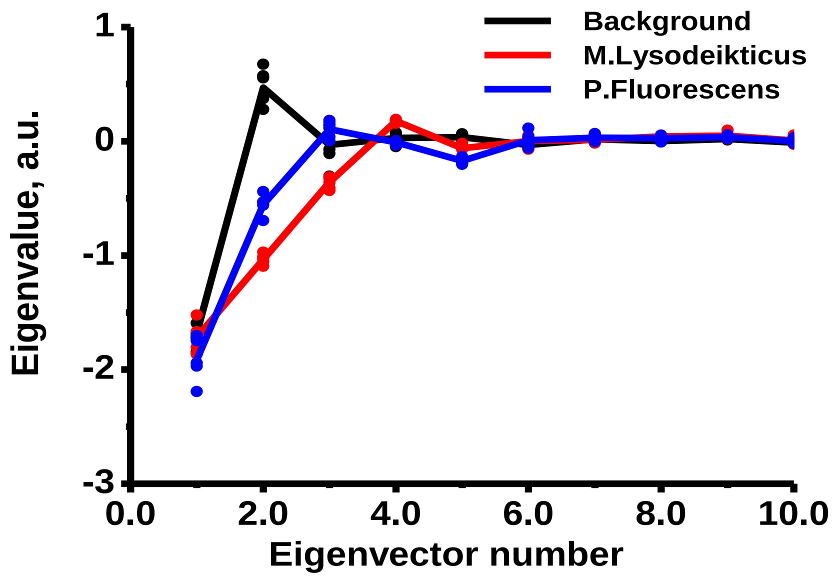
Micrococcus Lysodeikticus: Gram positive, spherical, aerobic bacterium
Pseudomonas Fluorescens: Gram-negative, rod-shaped, aerobic bacterium

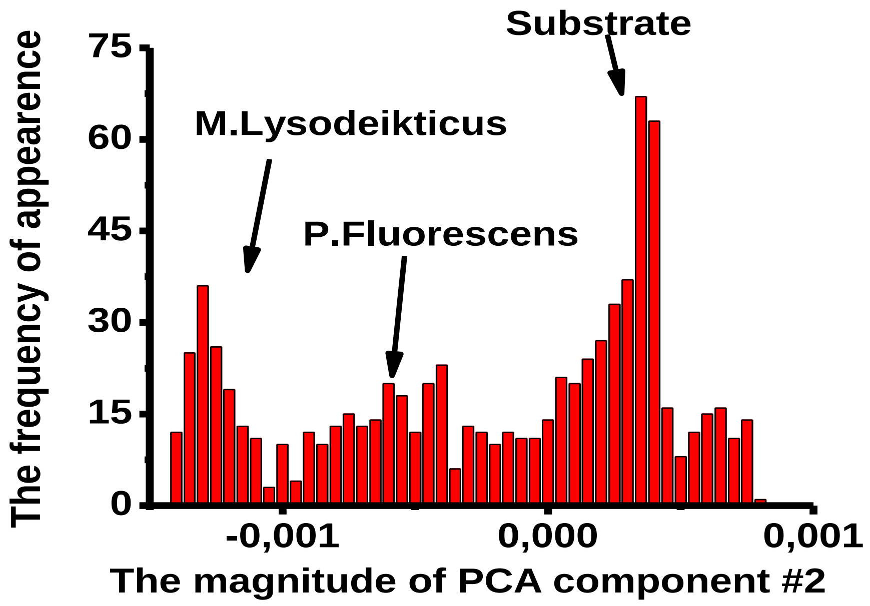
PCA separation?

Principal component analysis: $A_i(\omega_j) = a_{ik} w_k(\omega_j)$

$w_k(\omega)$ are found from $\mathbf{C} = \mathbf{A}\mathbf{A}^T$



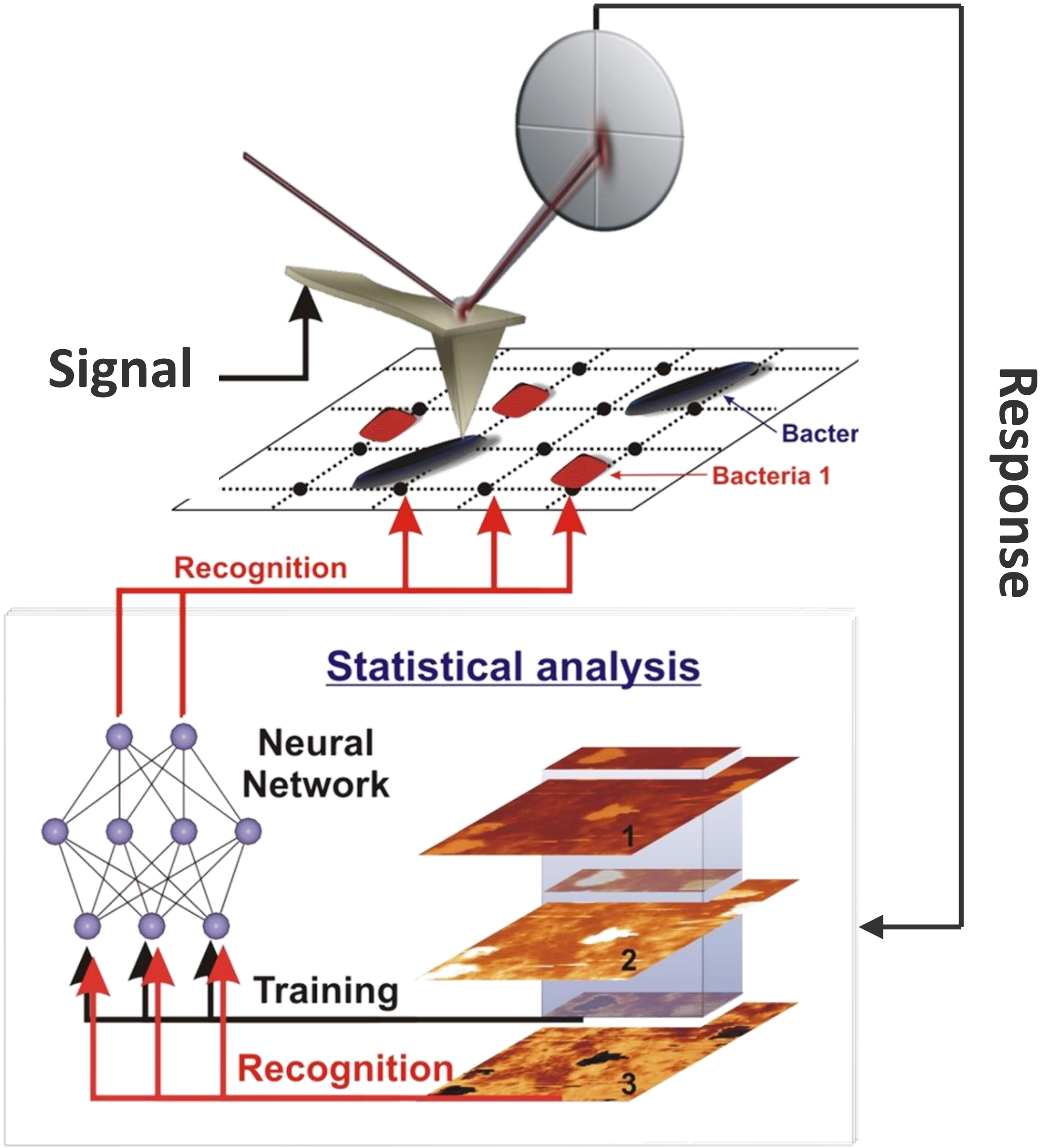




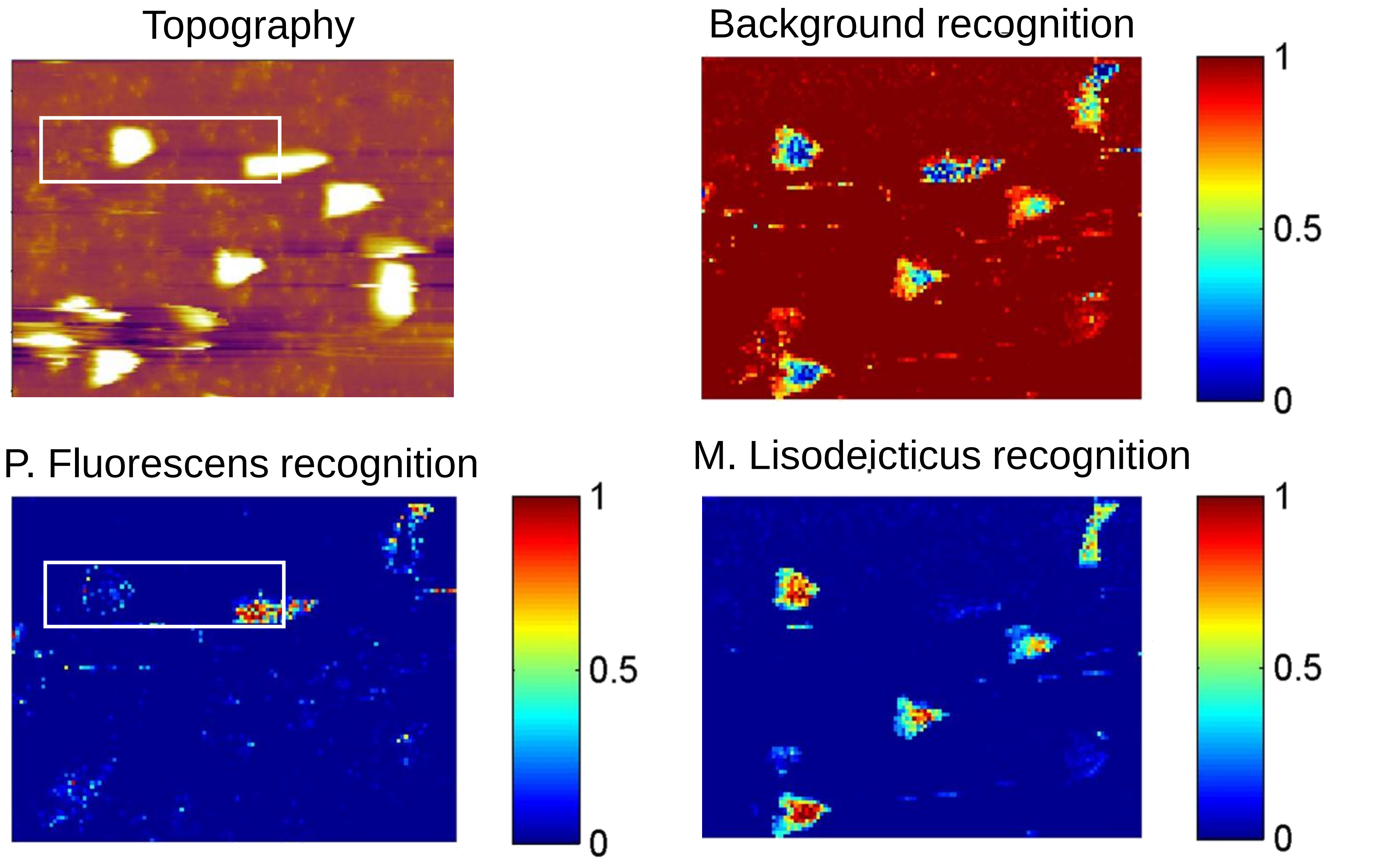
- Bacteria are differentiated on PCA maps
- One component is insufficient for unambiguous separation
- Need either shape information…
- Or all components!

Supervised bacteria identification

- Recognition imaging is implemented using BE PFM as signal
- However, any signal can be used: optical, mass-spectrometry, etc.
- Or any microscopic technique
- As long as labeled training set is available

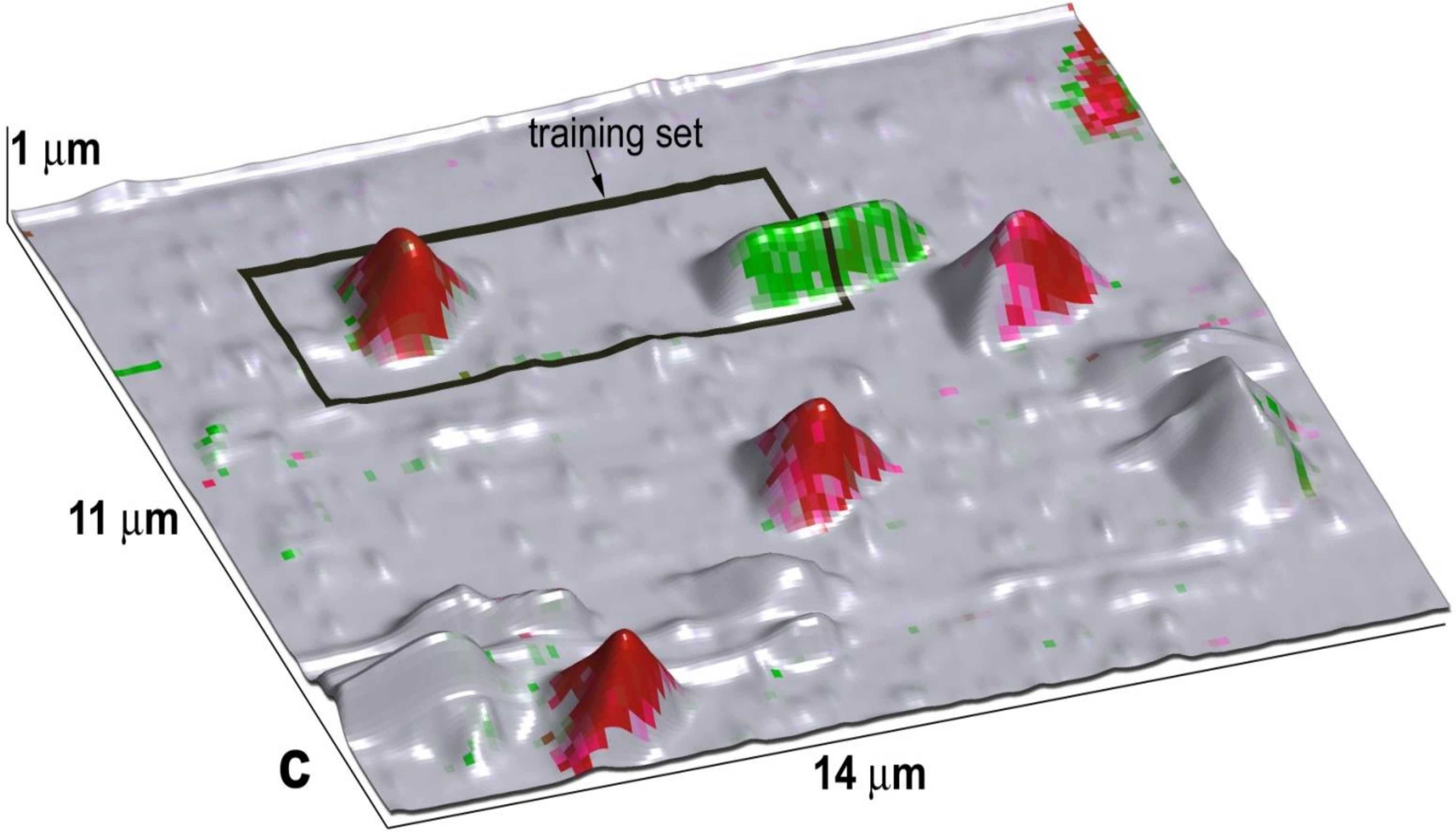


Recognition imaging of bacteria



M.P. NIKIFOROV, A.A. VERTEGEL, V.V. REUKOV, G.L. THOMPSON, S.V. KALININ, and S. JESSE, *Functional recognition imaging using artificial neural networks: Applications to rapid cellular identification by broadband electromechanical response*, Nanotechnology **20**, 405708 (2009).

Recognition imaging of bacteria



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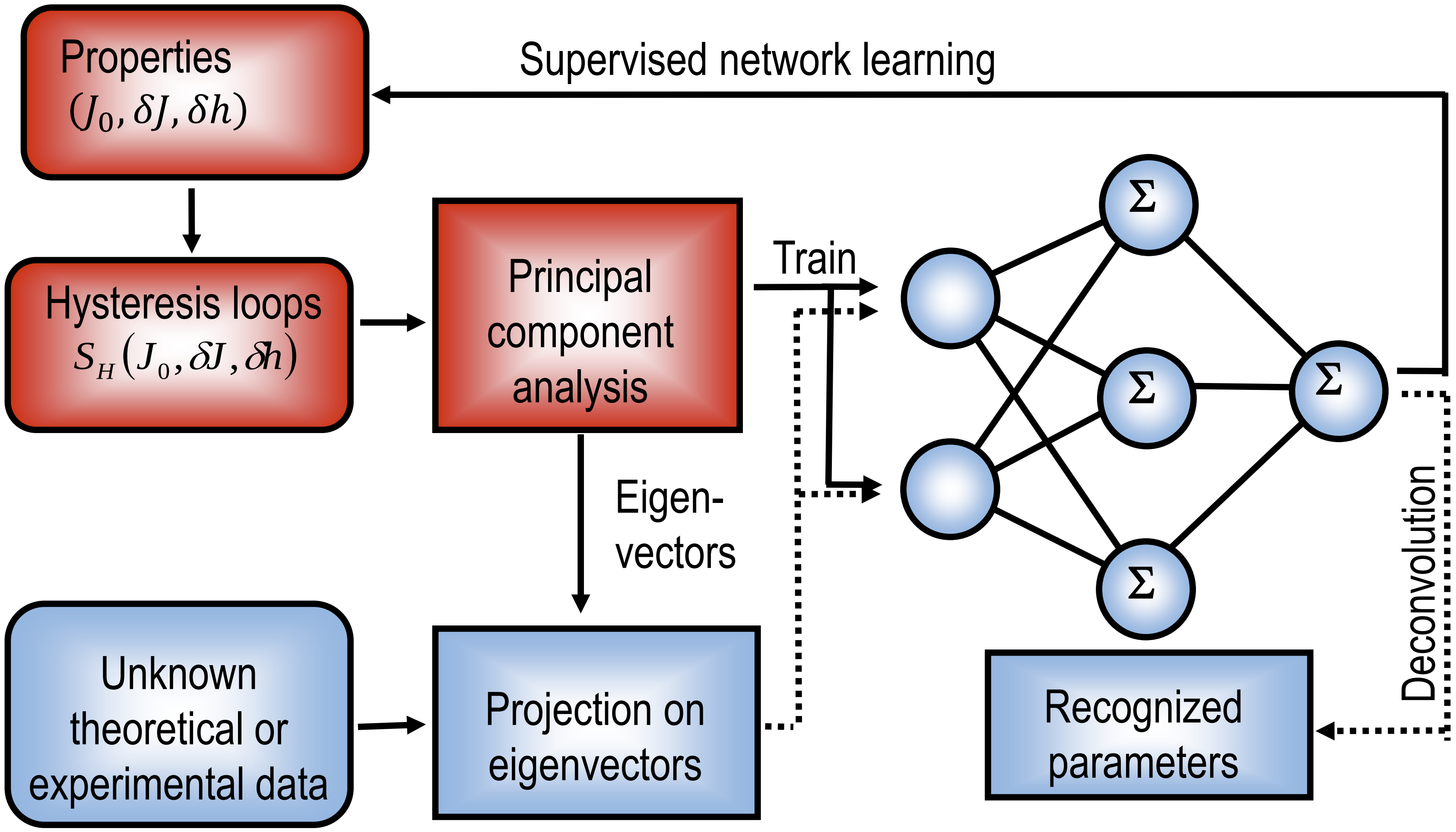
Can we train NN using model?



- A 'family' of Ising model-based hysteresis loops of varying parameters is calculated
- An artificial neural network is then trained to recognize each theoretical loop
- The trained neural network is then applied to experimental data to extract parameters

Ising model

Random bond – random field Ising model

Glauber dynamics

$$\mathrm{H}(H) = \sum_{i,j} J_{ij} S_i S_j + \sum_i (h_i + H) S_i$$

$$h_{loc}^i = \sum_j J_{ij} S_j - (H + h_i) \qquad h_{loc}^i S_i < 0$$

Figure by S. Jesse

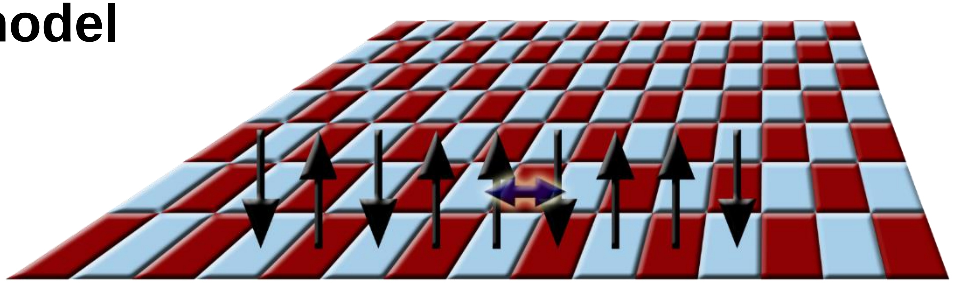
Relate hysteresis loops generated using the Ising model

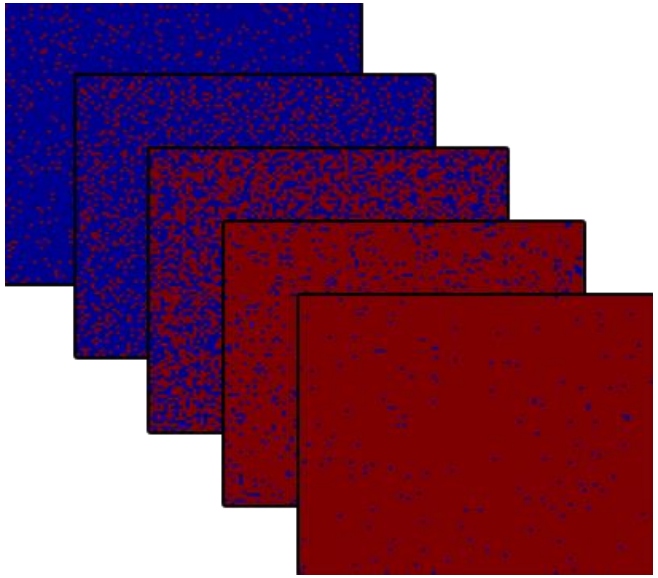
Exchange integral – J_0,

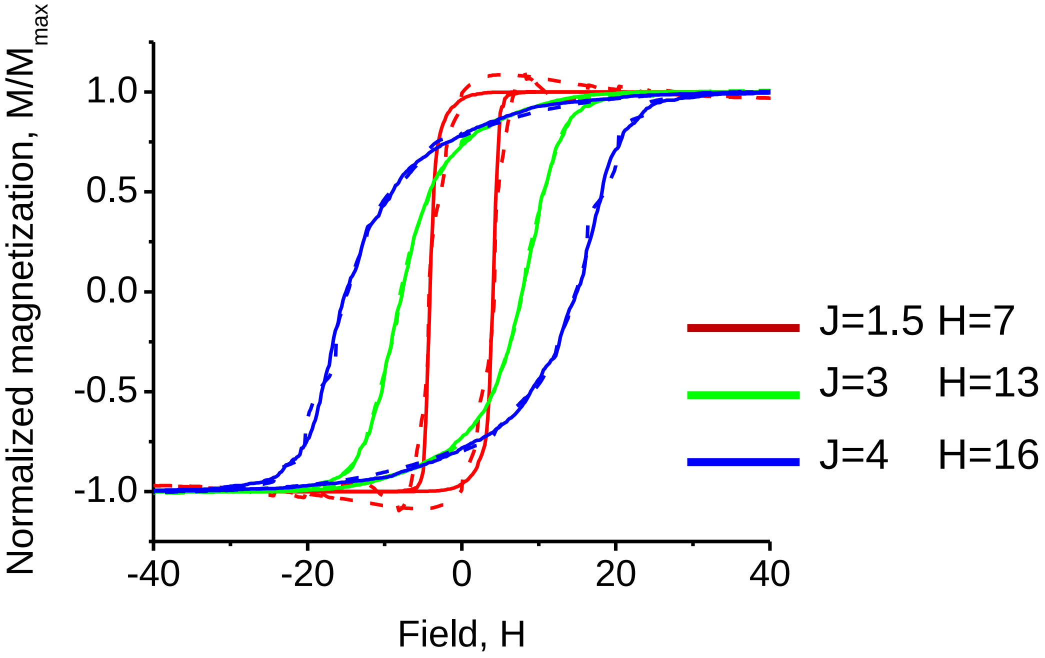
Random bond disorder - δJ,

Random field disorder - δh

to actual experimental ferroelectric switching loops

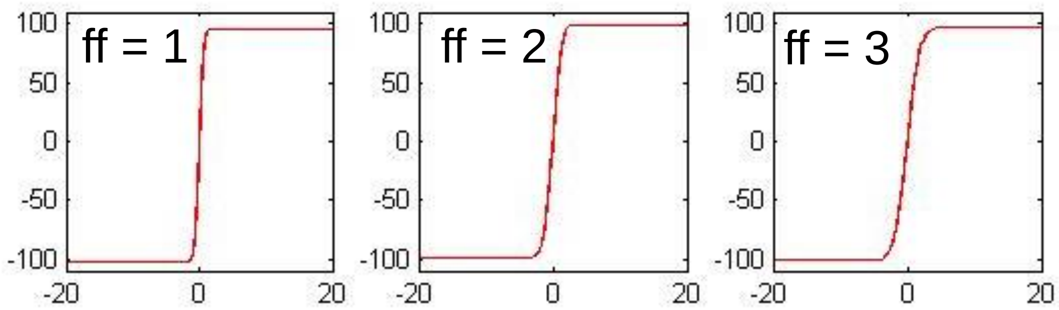




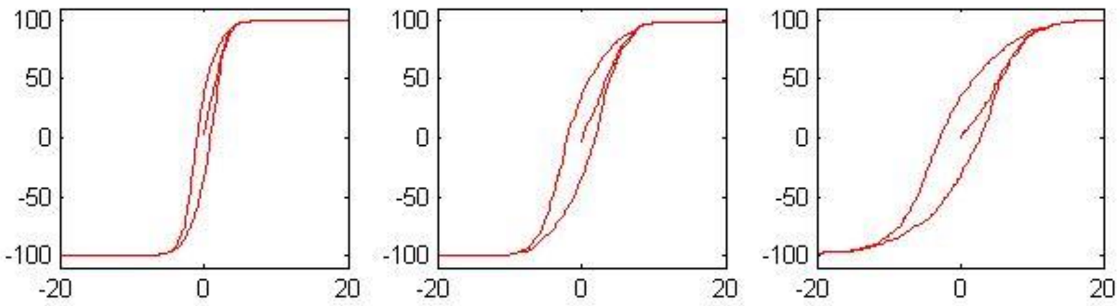


Examples:

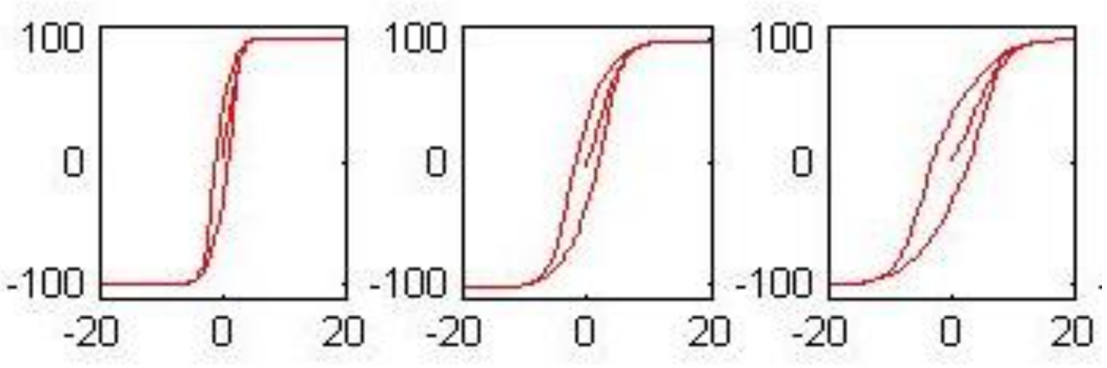
J_0 =0; δJ =0; δh =.5*ff;



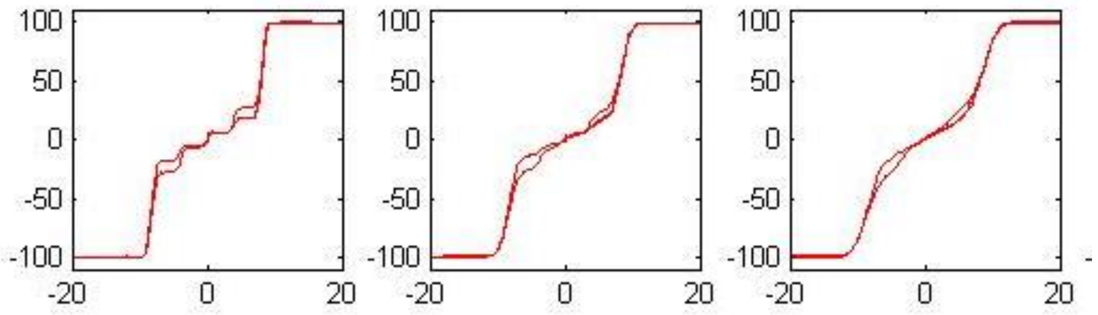
J_0 =0; δJ =.5*ff; δh =.5*ff;



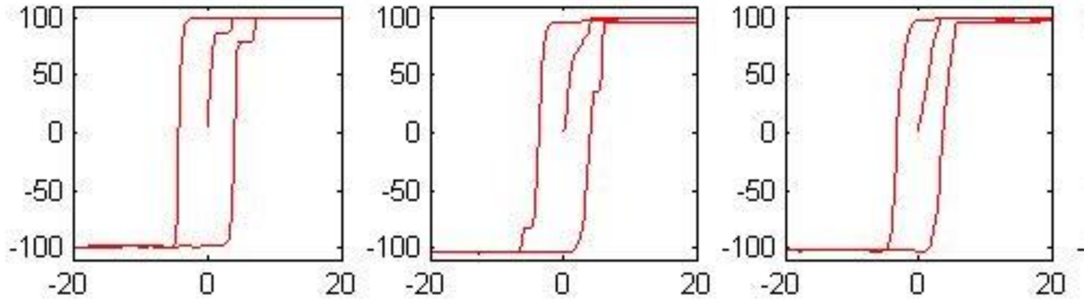
J_0 =0; δJ =.5*ff; δh = 0;



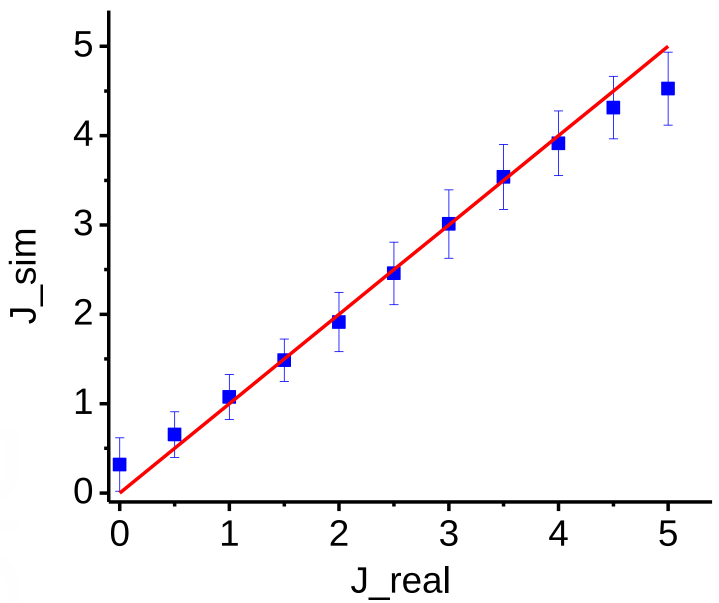
J_0 =-1; δJ =0; δh =.5*ff;

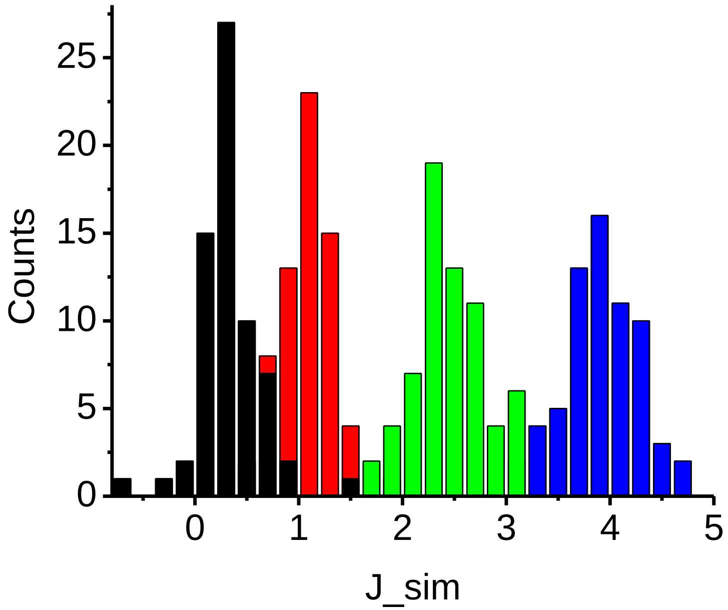


J_0 =1; δJ =0; δh =.5*ff;

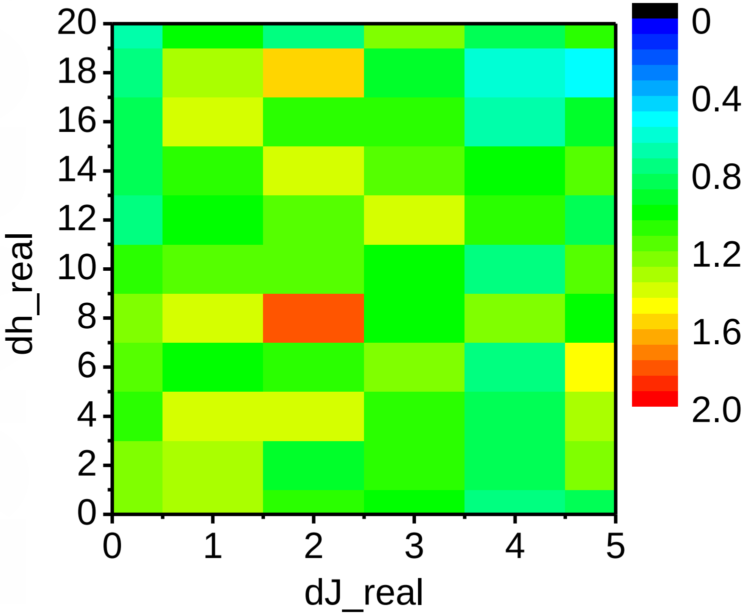


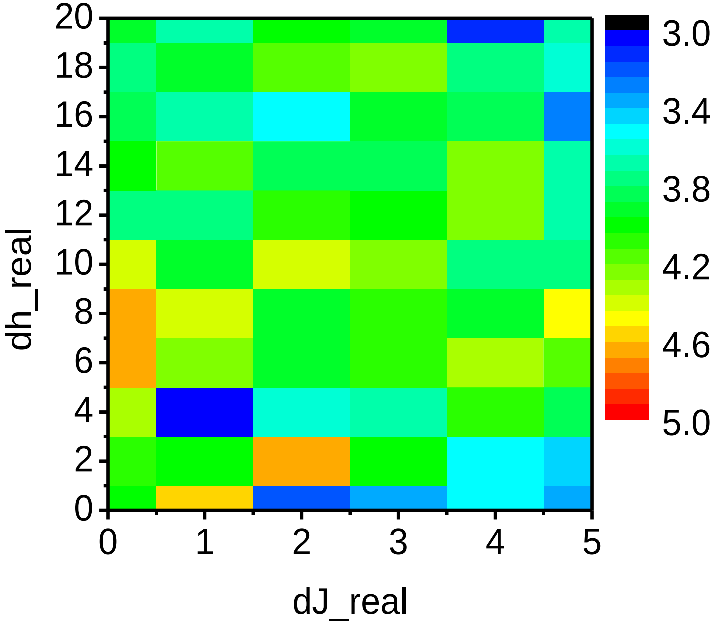
Self-recognition of Ising model



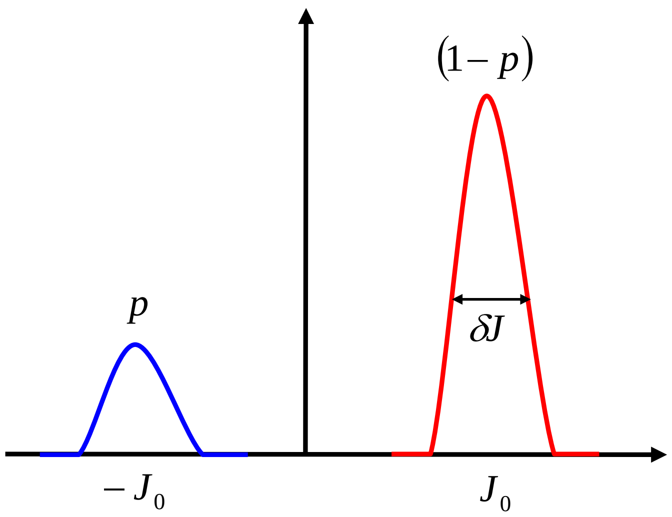


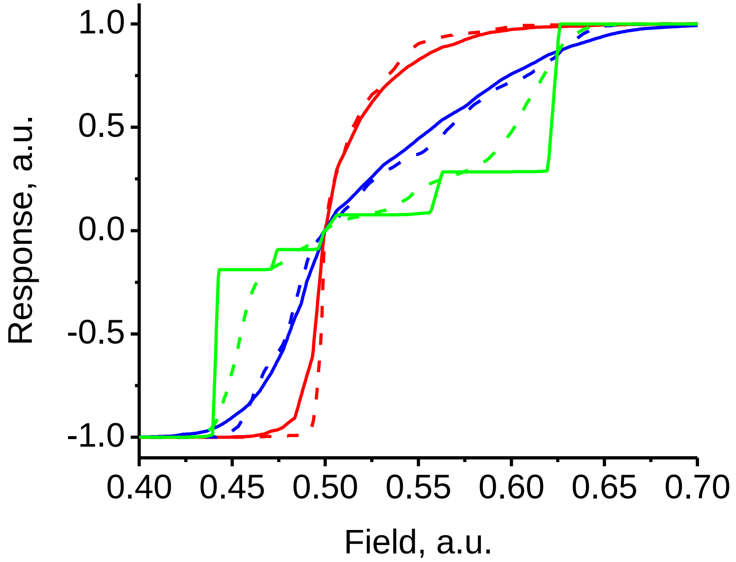
O.S. OVCHINNIKOV, S. JESSE, P. BINTACCHIT, S. TROLIERMCKINSTRY, and S.V. KALININ, *Disorder identification in hysteresis data: recognition analysis of random-bond random-field Ising model*, Phys. Rev. Lett. **103**, 157203 (2009).





Recognition of more complex model





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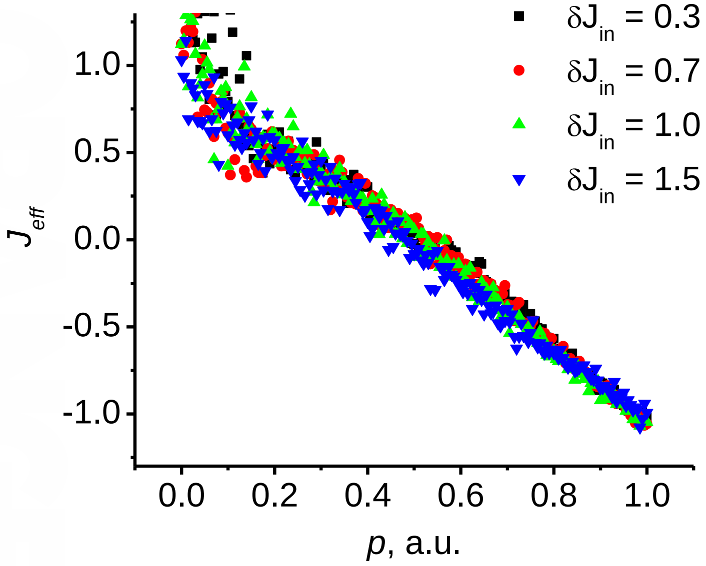
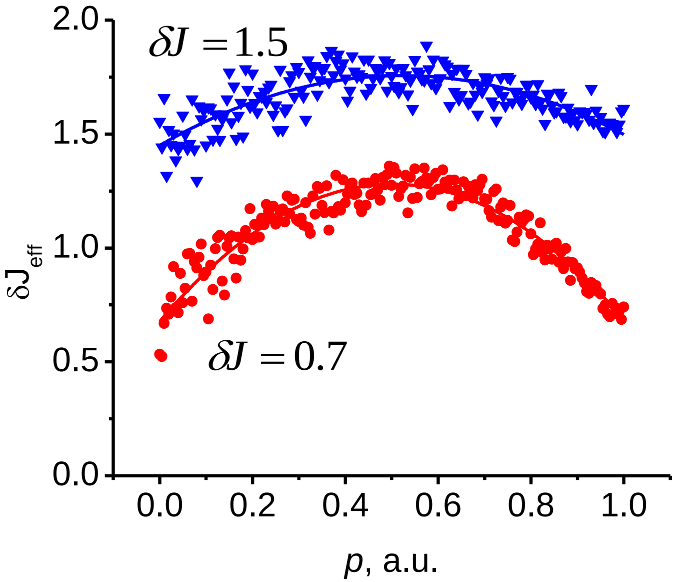
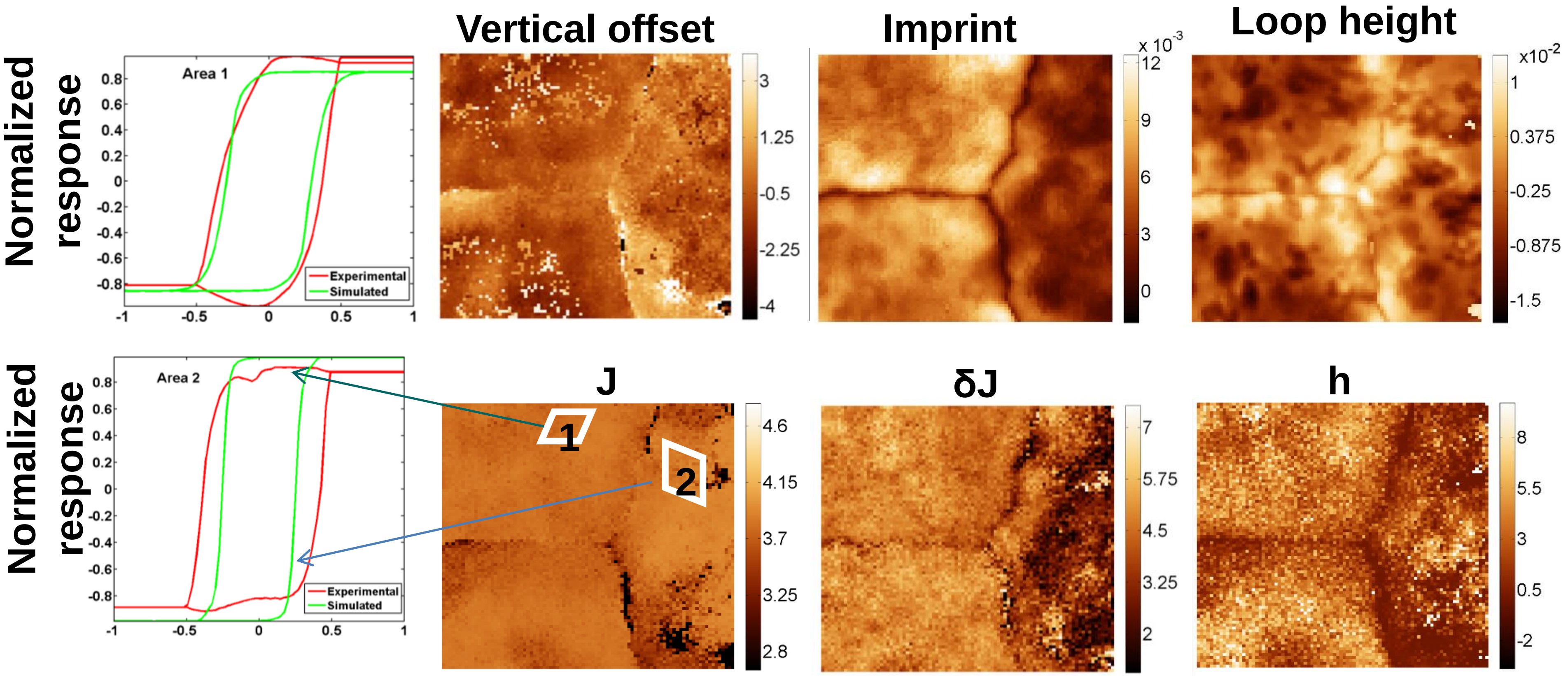




Analysis of loops based on Ising model



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A. KUMAR, O. OVCHINNIKOV, S. GUO, F. GRIGGIO, S. JESSE, S. TROLIER-MCKINSTRY, and S.V. KALININ, *Spatially Resolved Mapping of Disorder Type and Distribution in Random Systems using Artificial Neural Network Recognition*, Phys. Rev. **B 84**, 024203 (2011).

Convolutional neural network (CNN)

• Convolutional Neural Networks (CNNs) are a class of deep learning models, applied to analyzing visual imagery.
•CNNs are invariant to object position and distortion in the scene.
•CNNs use fewer parameters than fully connected networks, which makes them computationally efficient.

Two major components of CNN:

- Convolutions (kernel size, stride, and padding):
  - Filter or "kernel“ (learnable parameters is passed over the input data
  - Performs element-wise multiplication and sums up the results to produce a transformed version of the input (feature map)
- Pooling (subsampling or downsampling):
  - Used to reduce the dimensionality of the feature map
  - Min, max, and mean are the most commonly used.

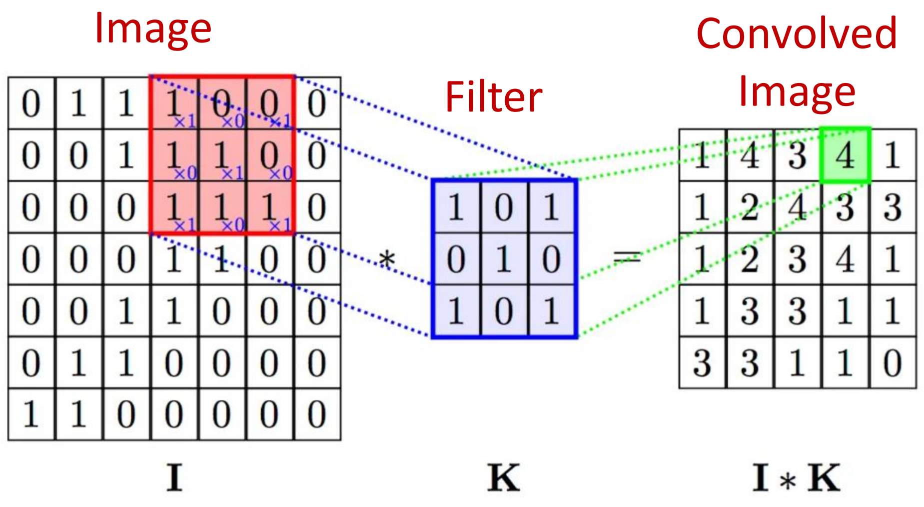
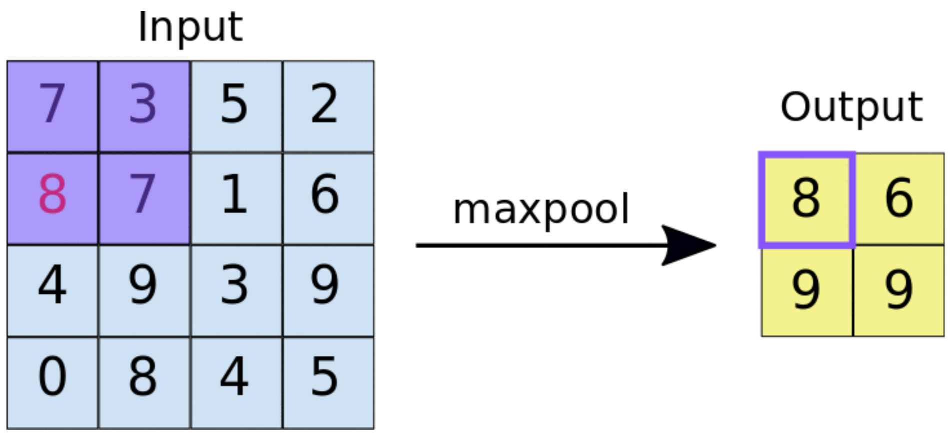


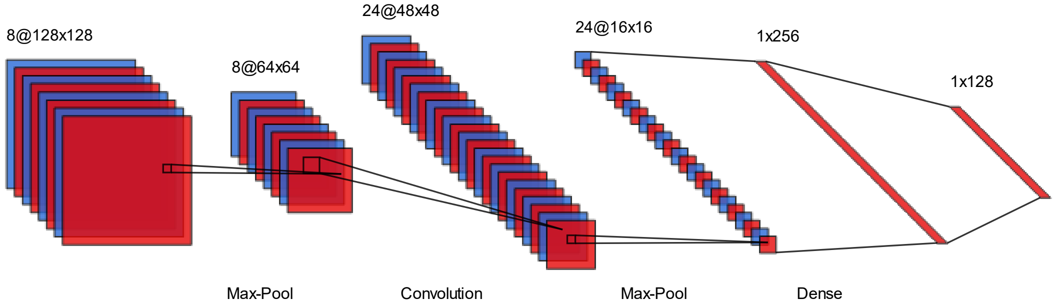
Image convolution



Max pooling layer

Deep convolutional neural network (DCNN)

- DCNNs are specialized kind of neural networks that are particularly effective for image processing tasks.
- The neurons in each layer are only connected to a small region of the previous layer, imitating the receptive fields of neurons in the human visual cortex.
- DCNNs consist of a series of convolutional layers, followed by non-linear activation functions, and often pooling layers to downsample the data.
- These layers can learn to detect low-level features such as edges and curves, while deeper layers can recognize higher-level features like shapes or specific objects.
- The final layers of a DCNN are typically fully connected layers, which perform classification/regression based on the features learned by the preceding convolutional layers.
- DCNNs are integral to a range of specific applications including image and video classification, object detection, semantic segmentation, instance segmentation, image restoration, and even style transfer in images and videos.



AlexNet

Semantic segmentation and image labeling

• Semantic segmentation classifies each pixel image into one of pre-defined number of classes.

•This is different from the typical image classification where the image is classified as a dog or no-dog image

• The targets for the semantic segmentation task are usually hand drawn using tools like imageJ.

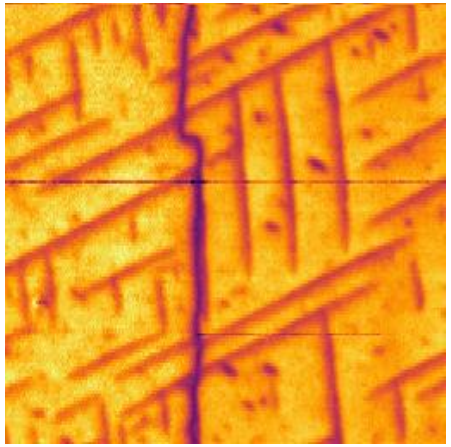
•One way to overcome this is to create synthetic images that represent the real-world dataset.

- In synthetic datasets, the interesting objects can be placed in predefined positions and orientations.
- A deep neural network that is trained on the synthetic dataset and can later be used to semantically segment the real-world dataset.
- It is essential that we capture all the data variances in the real-world dataset and incorporate them in the synthetic dataset or else this would not work.
- Tools in atomai assist you in creating proxies for atomically resolved electron microscopy images. (More on that later).

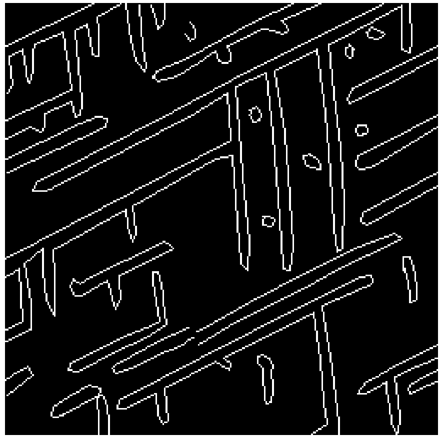
Semantic segmentation *vs.* image classification

Dog

Semantically segmented cat



Raw PFM data

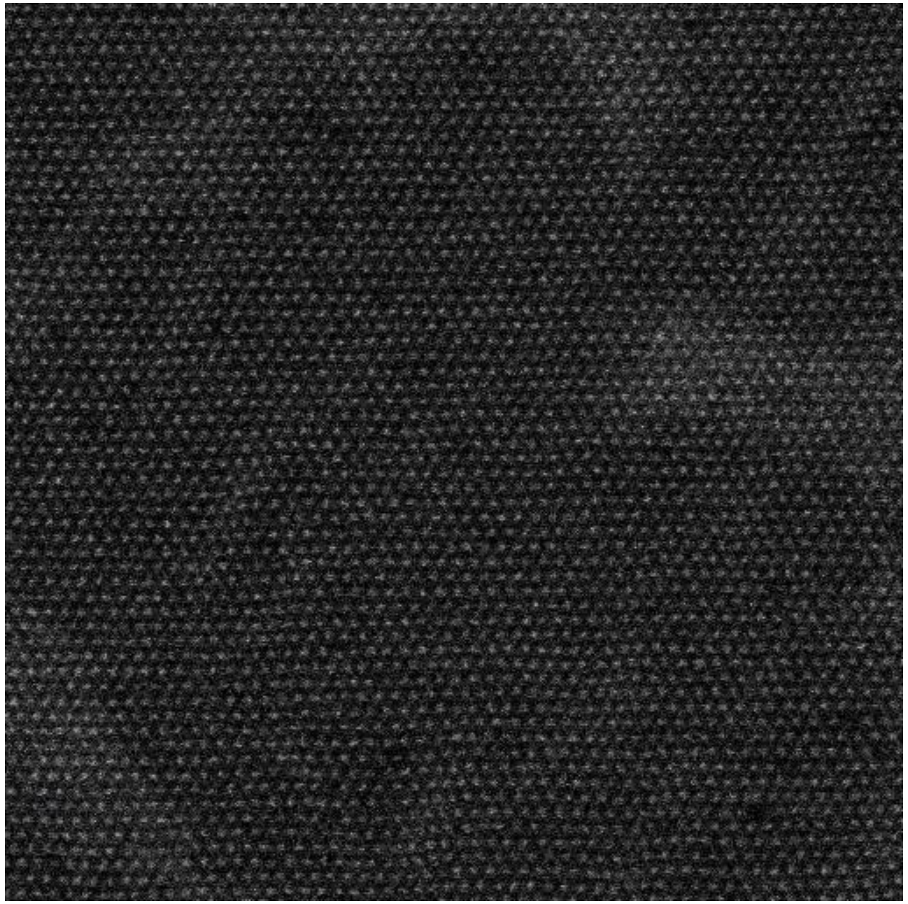


Domain walls hand-drawn using imageJ

Labeling datasets for semantic segmentation

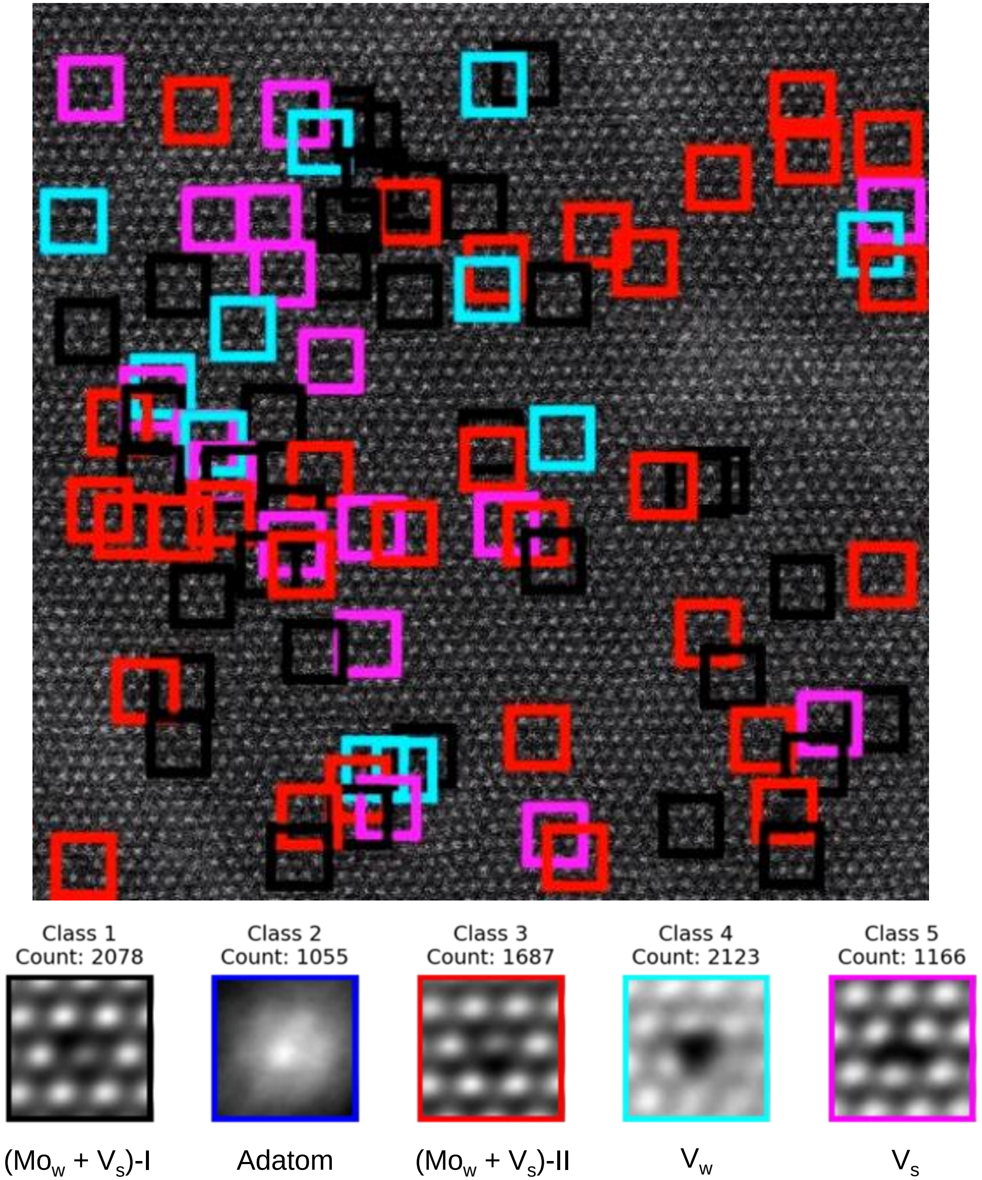
Learning the defect evolution

Experimental



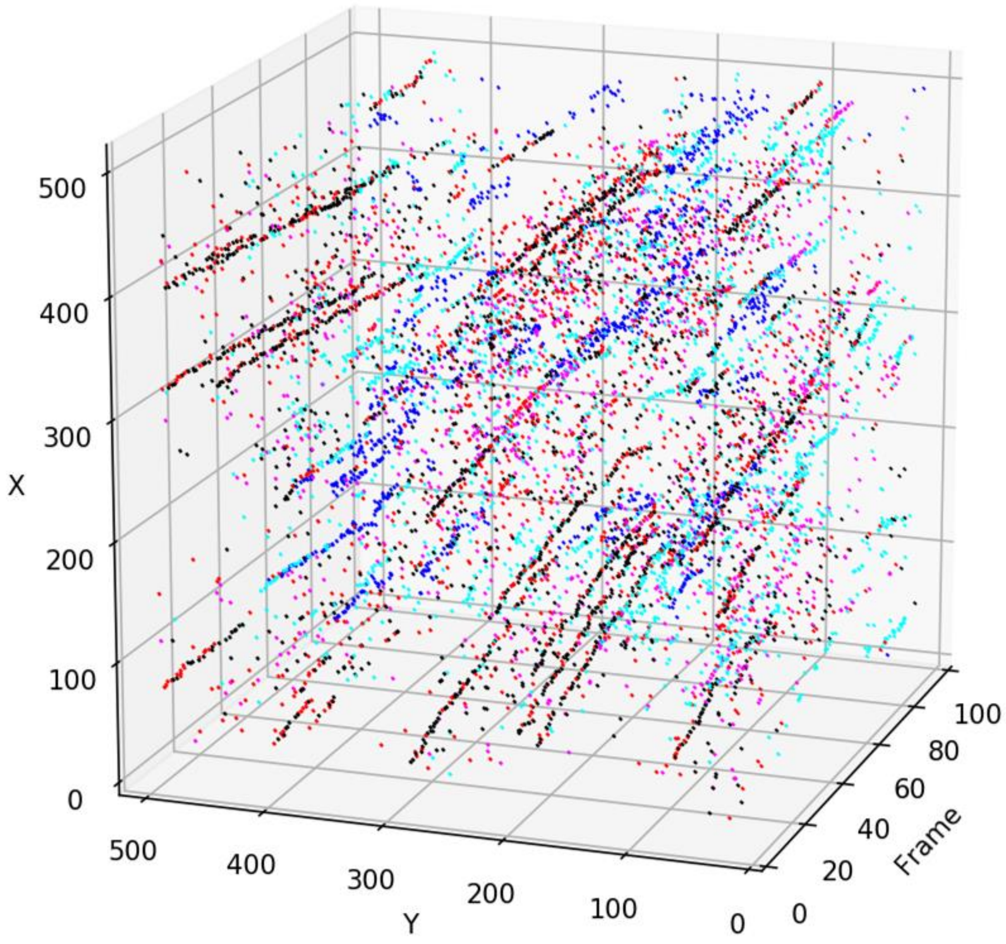
Sample: WS_2, E-beam energy: 60 kV
Data collected by Ondrej Dyck (CNMS/ORNL)

Decoded



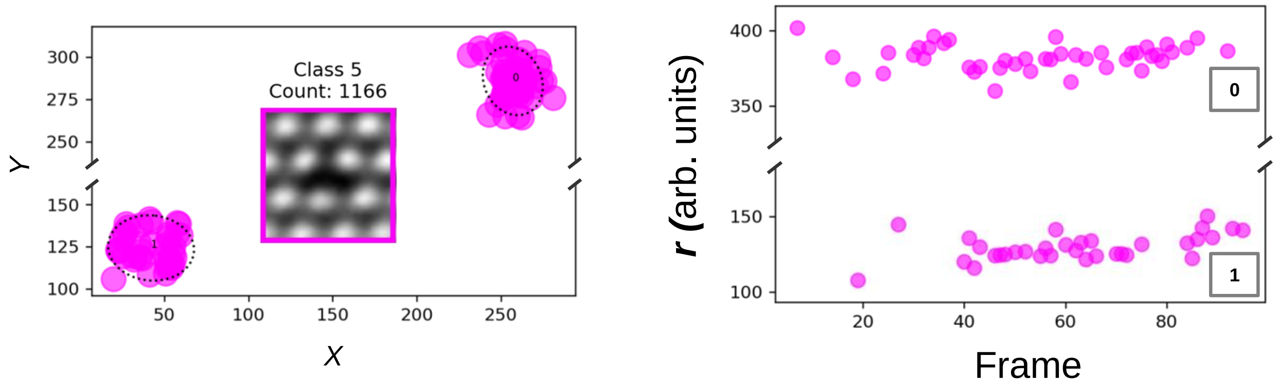
Exploring defect dynamics

Spatio-temporal trajectories



Maksov *et al.*, npj Comp. Mat. **5**, 12 (2019)

Diffusion parameters for selected defect types

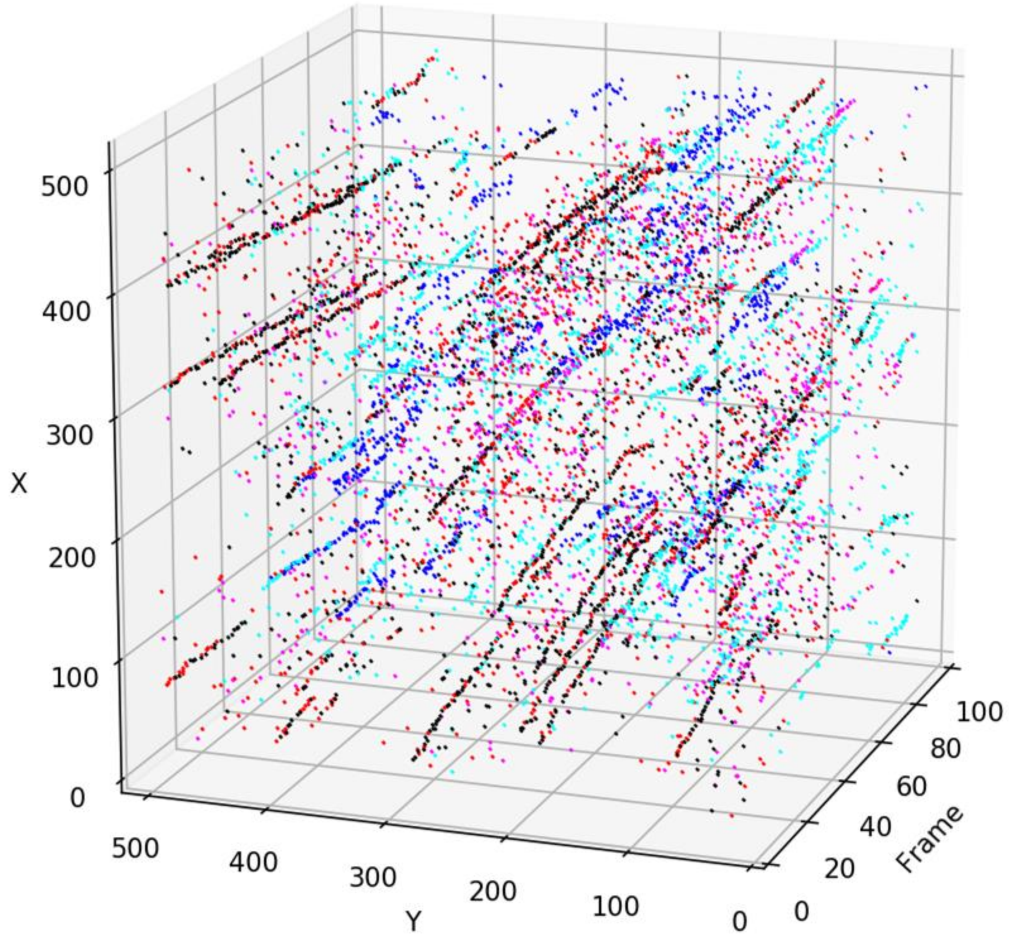


Diffusion coefficient: 3×10^{-4} nm^2/s - 6×10^{-4} nm^2/s (within 2D random walk approximation)

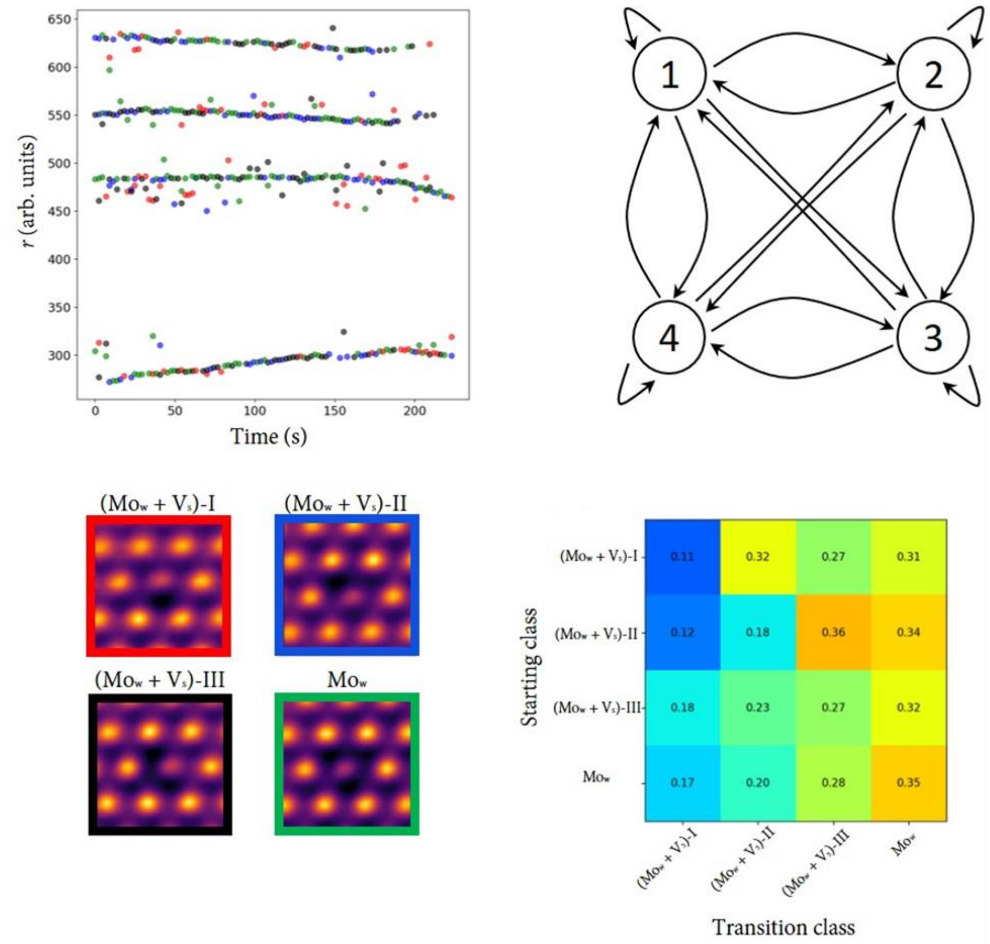
- Identification of dominant point defects and their characteristic statistical behaviors
- Analysis of diffusion parameters for the selected defect species
- Study of transformation pathways and transition probabilities for composite defects

Exploring defect dynamics

Spatio-temporal trajectories

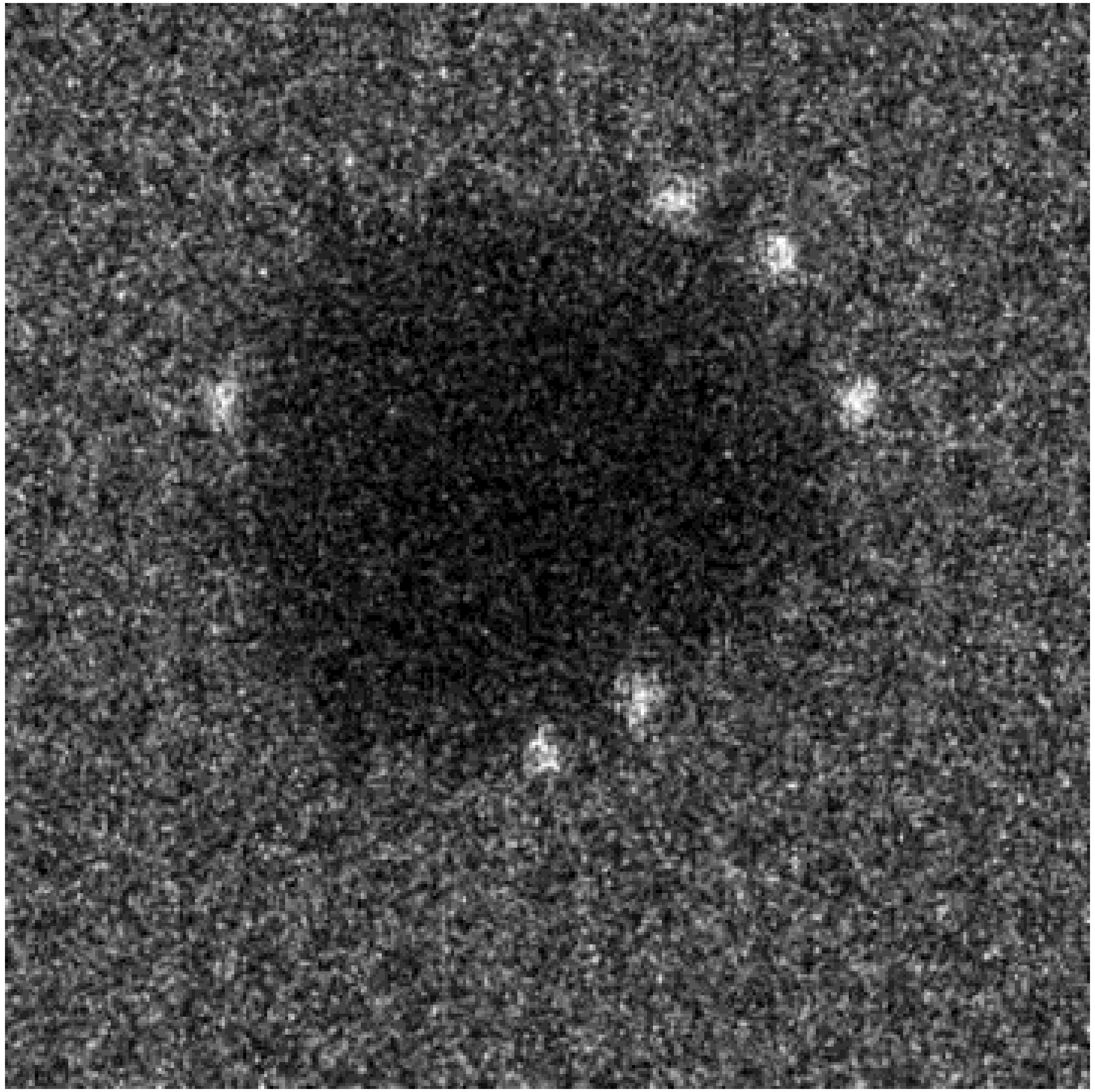


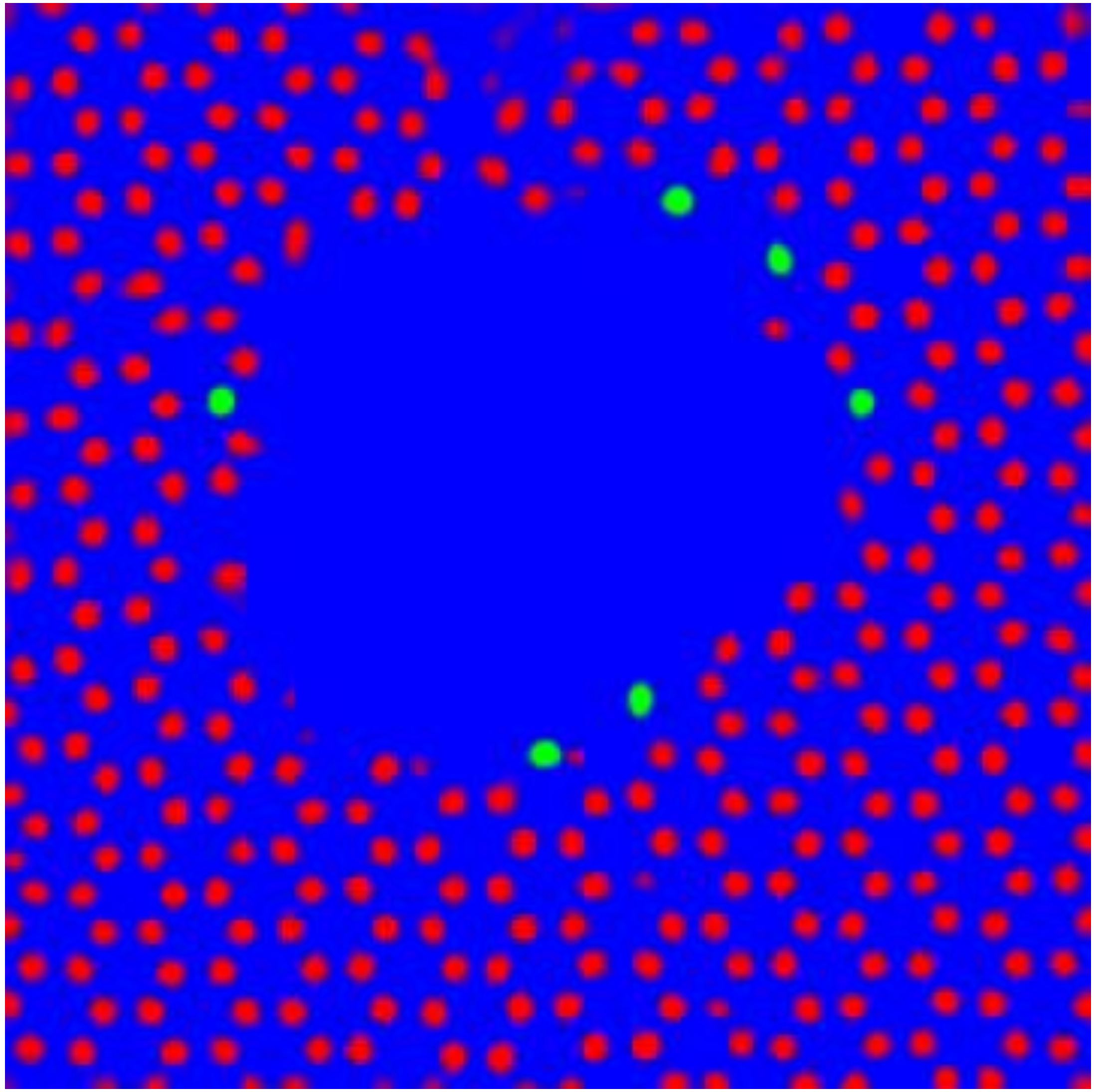
Evolution of defects as Markov process



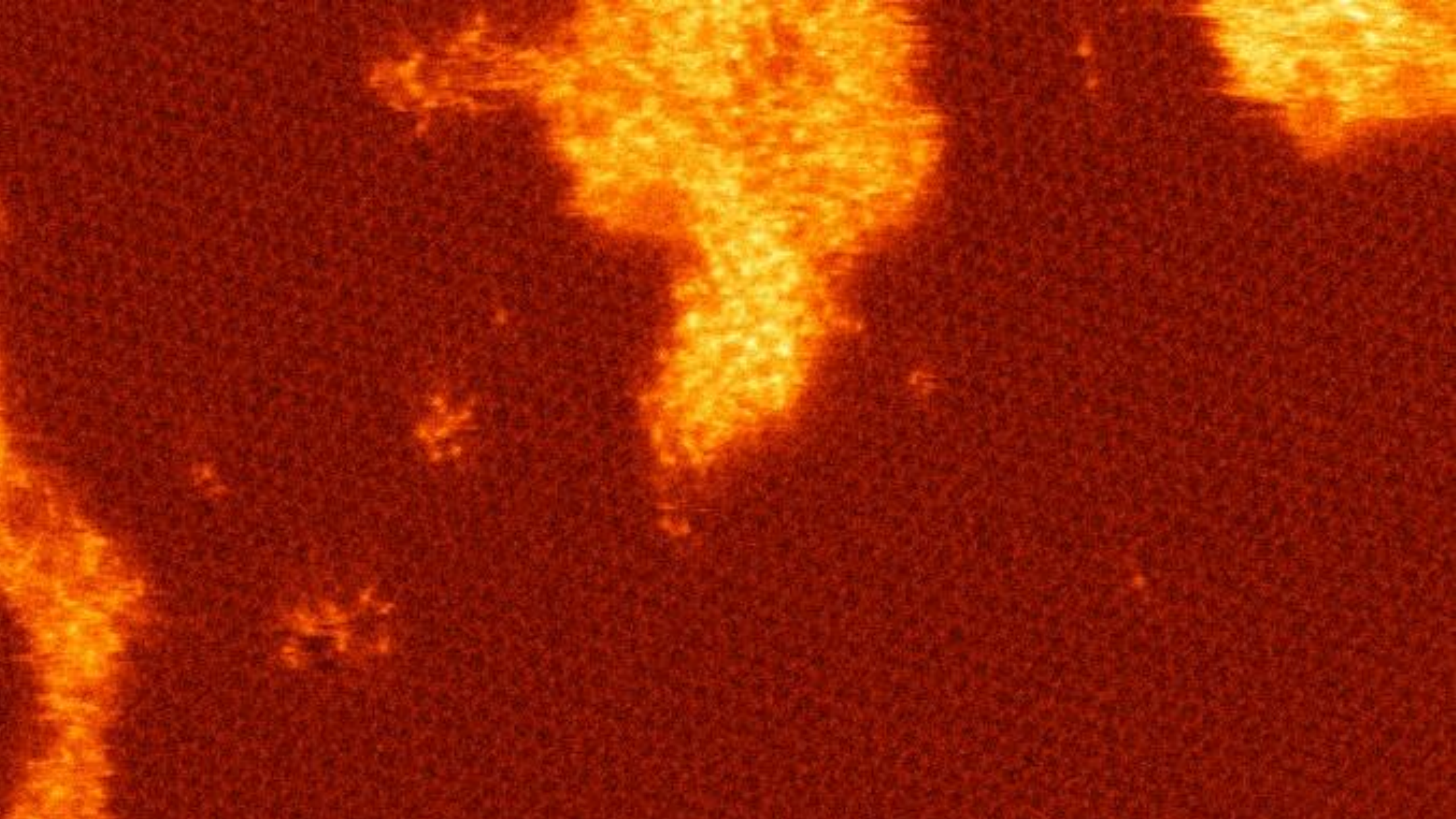
Maksov *et al.*, npj Comp. Mat. **5**, 12 (2019)

Deep learning for atom finding

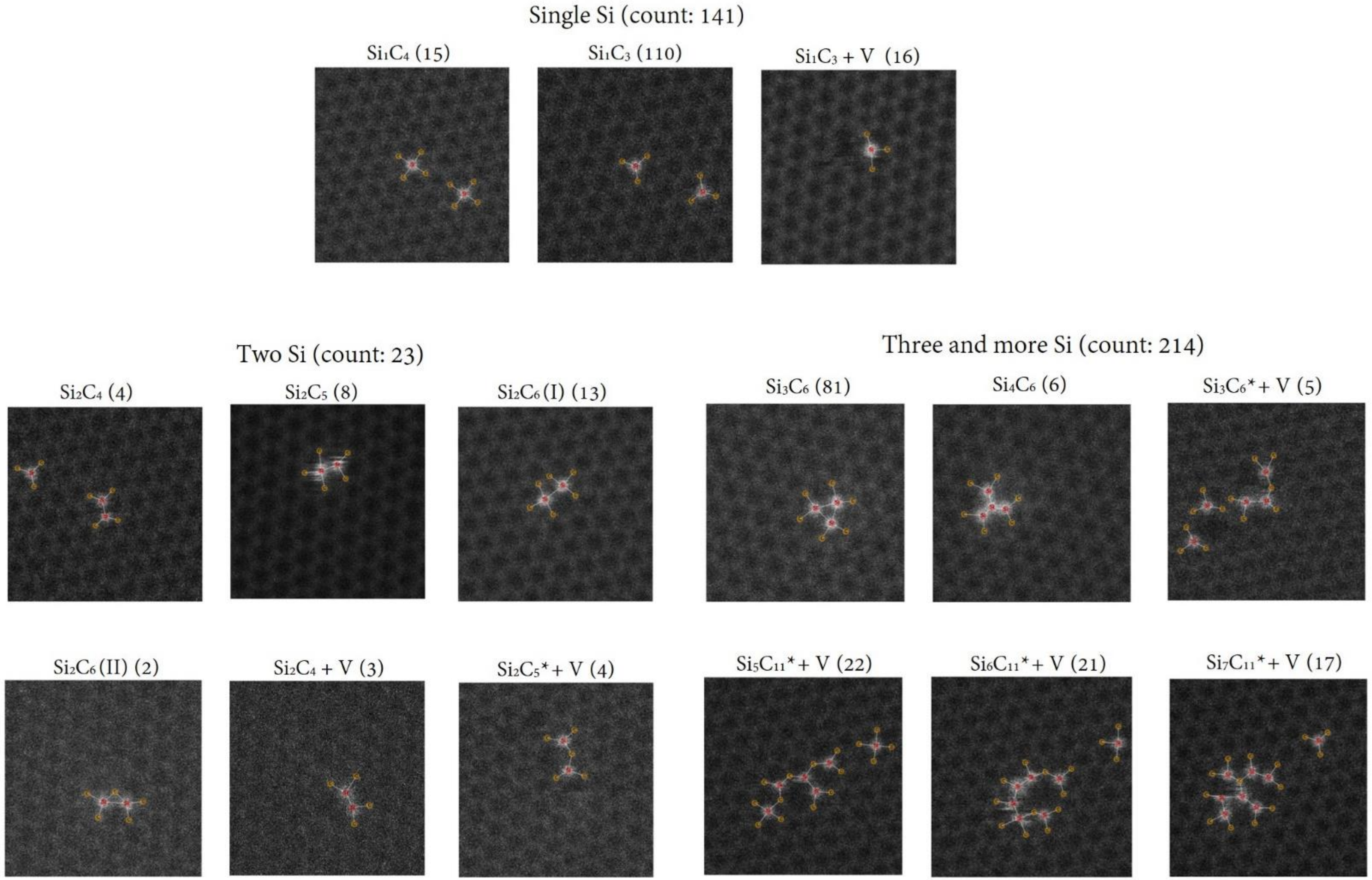




M. Ziatdinov, ACS Nano 2017



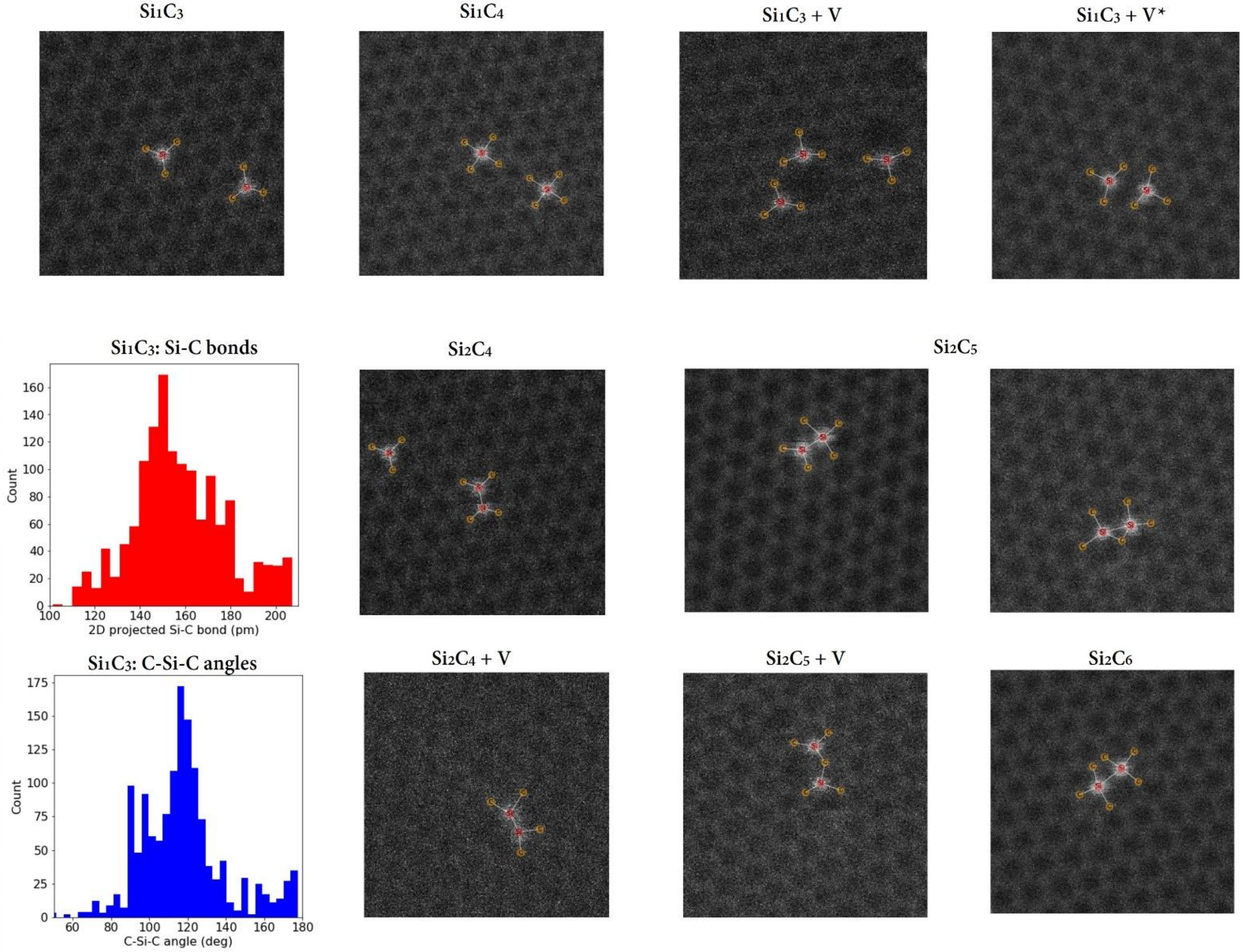
Defect libraries



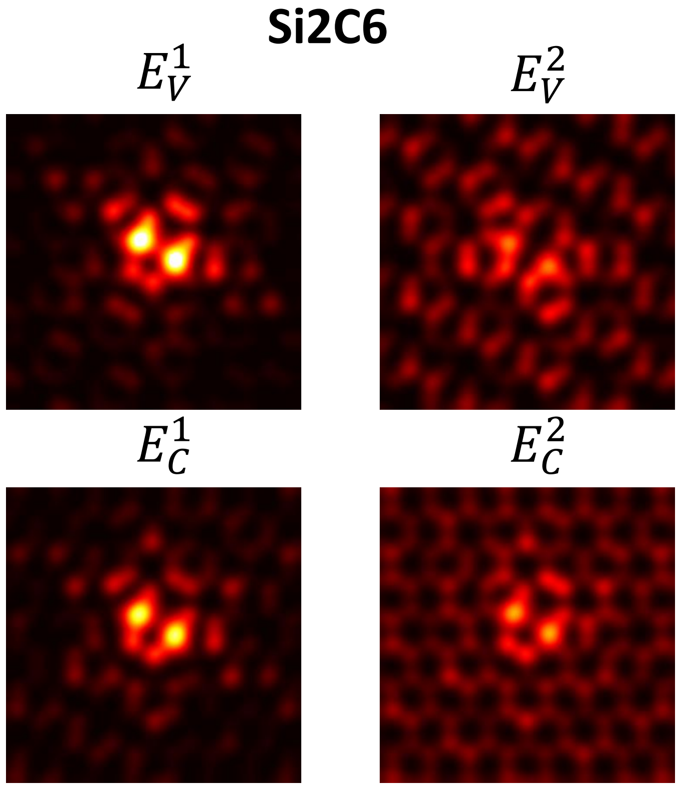
To create libraries of defects in graphene, we used active manipulation via 100 kV electron beam to disperse Si impurities over graphene lattice. The automated image analysis and recognition based on the deep learning networks is developed to identify and enumerate the defects

Augmented defect libraries

Creation of Si-vacancy libraries from STEM data



Adding electronic structure calculations to library

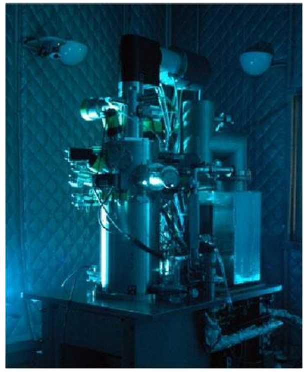


M. Ziatdinov *et al.* ArXiv:1809.04256 (2018).

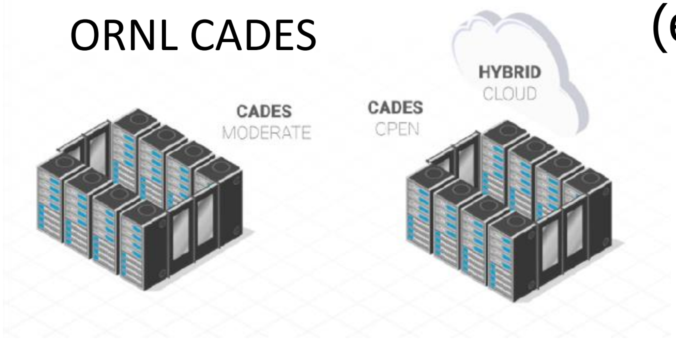
Total number of images analyzed: ~600 (ranging from 256 × 256 to 2048 × 2048 and from 2 nm × 2 nm to 16 nm × 16 nm)

Applications of defect libraries

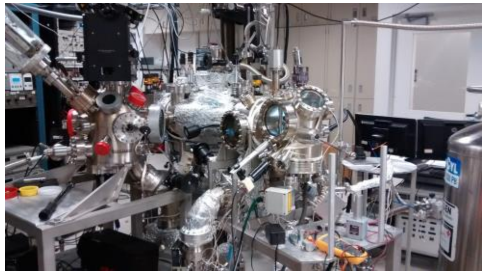
Scanning Transmission Electron Microscope (STEM) (structure)



ORNL CADES

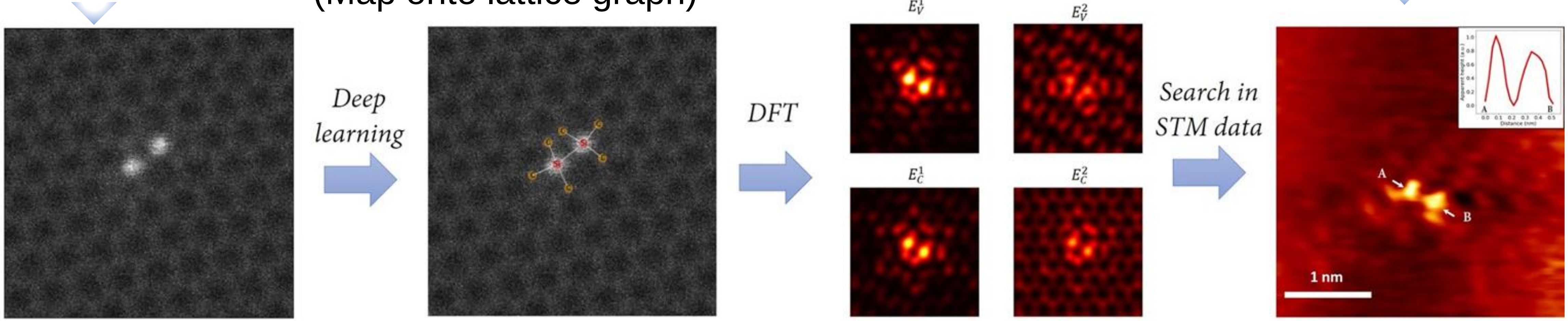


Scanning Tunneling Microscope (STM) (electronic properties)



Identification of new defects (Map onto lattice graph)

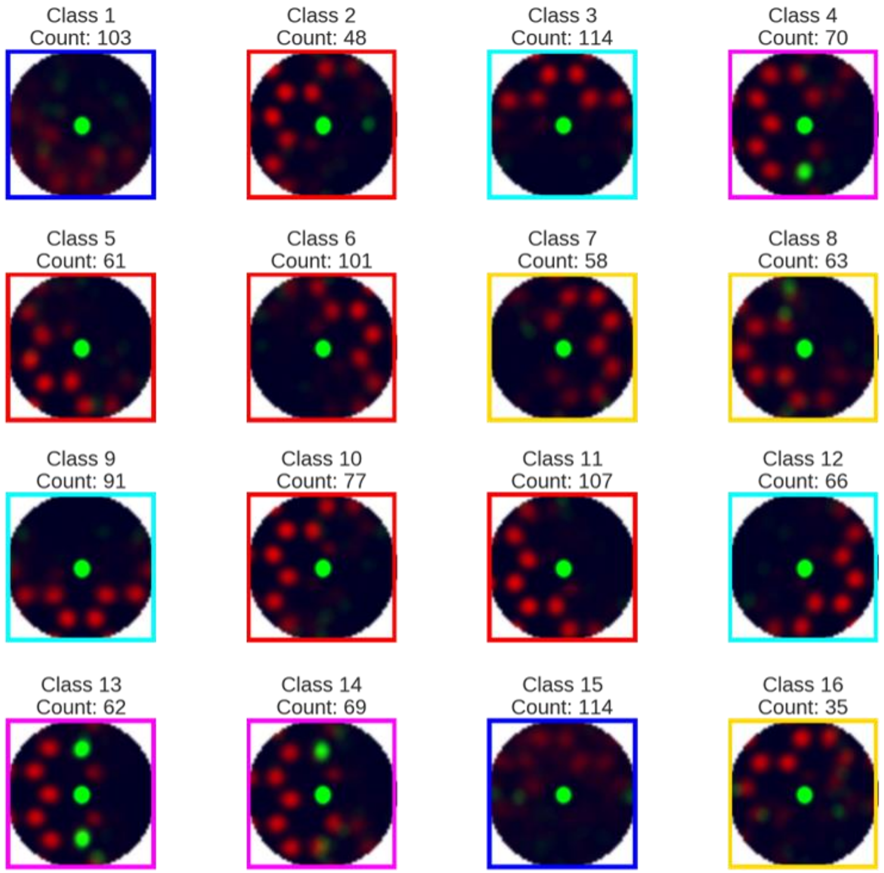
Calculated electronic structure



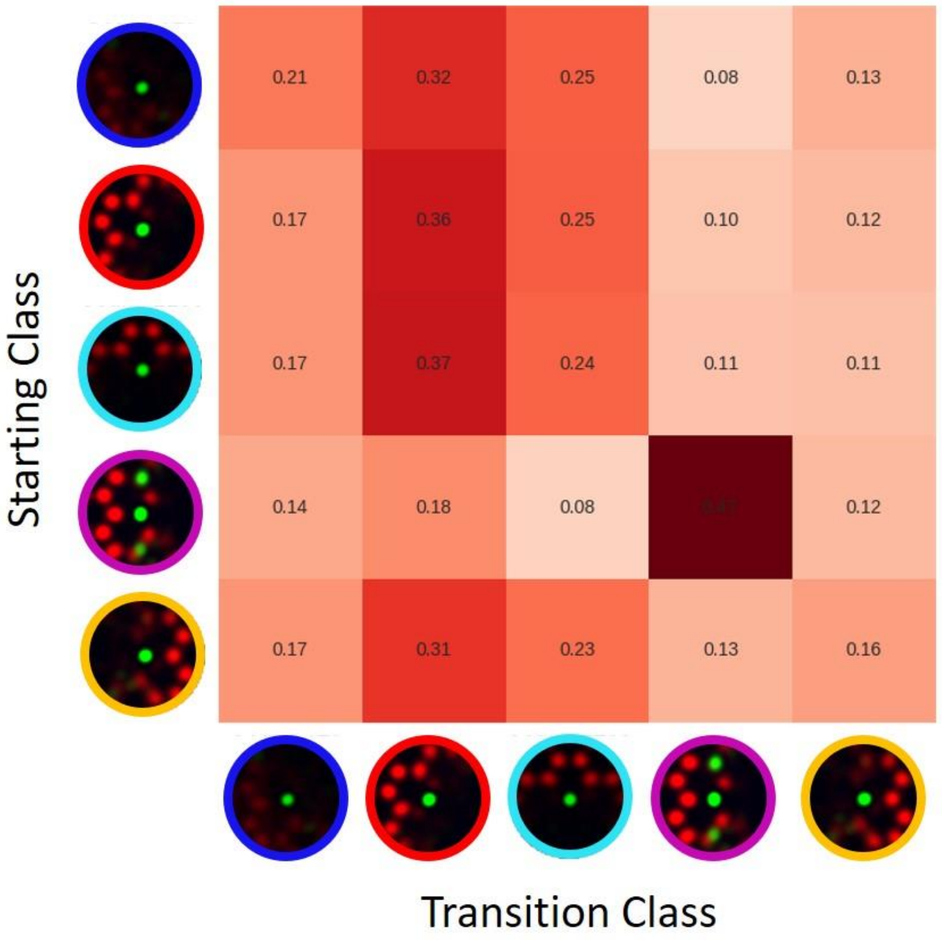
M. Ziatdinov, O. Dyck, B. G. Sumpter, S. Jesse, R. K. Vasudevan, S. V. Kalinin. *Building and exploring libraries of atomic defects in graphene: scanning transmission electron and scanning tunneling microscopy study*. ArXiv:1809.04256 (2018)

Structural elements

Derived classes of Si-C edge configurations



Transition probabilities matrix

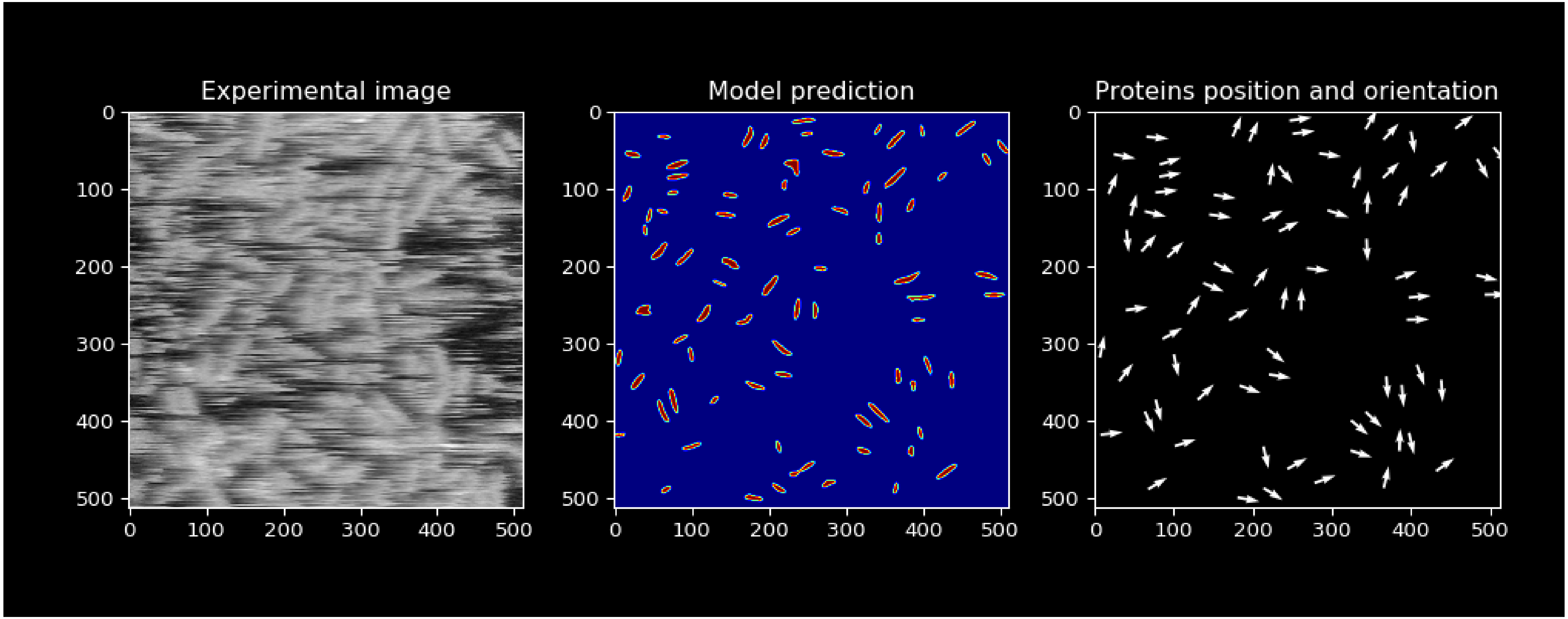


- Gaussian mixture model
- Discrete rotation symmetry + structural similarity algorithm
- Markov state analysis

Ziatdinov *et al*., ArXiv:1901.09322 (2019)

Deep learning in mesoscopic imaging

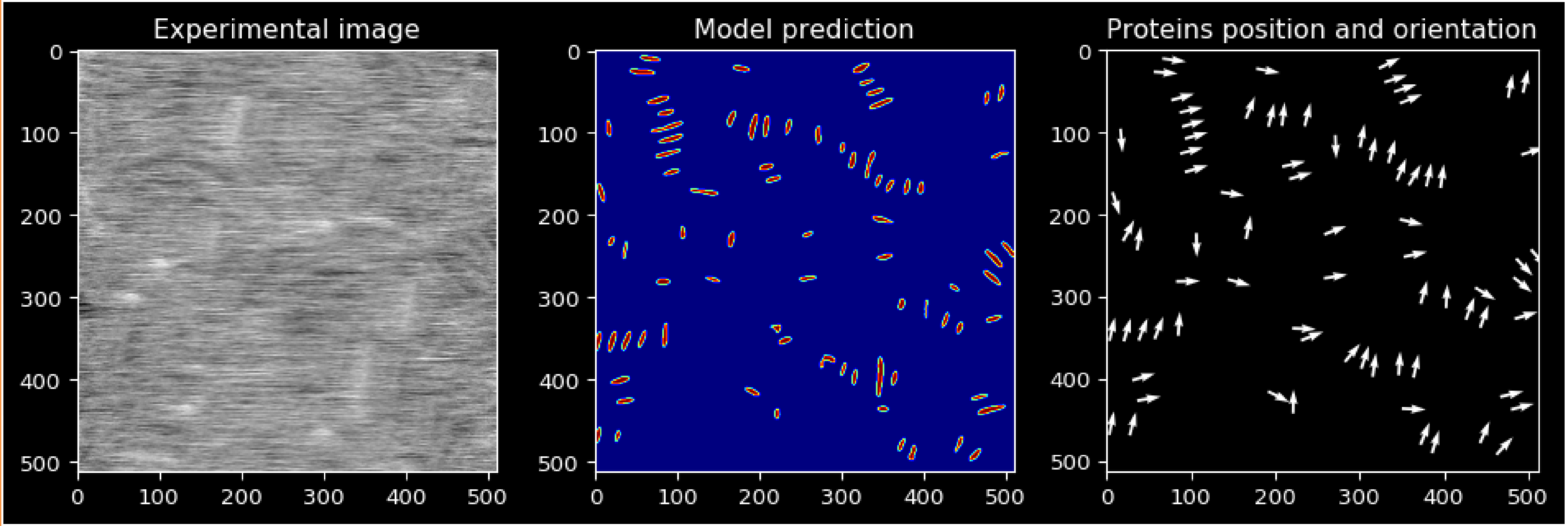
Model trained on a single movie frame from the well-ordered phase and applied to the entire movie



Maxim Ziatdinov, Xin Li, Shuai Zhang, Harley Pyles, David Baker, James J. De Yoreo, Sergei V. Kalinin

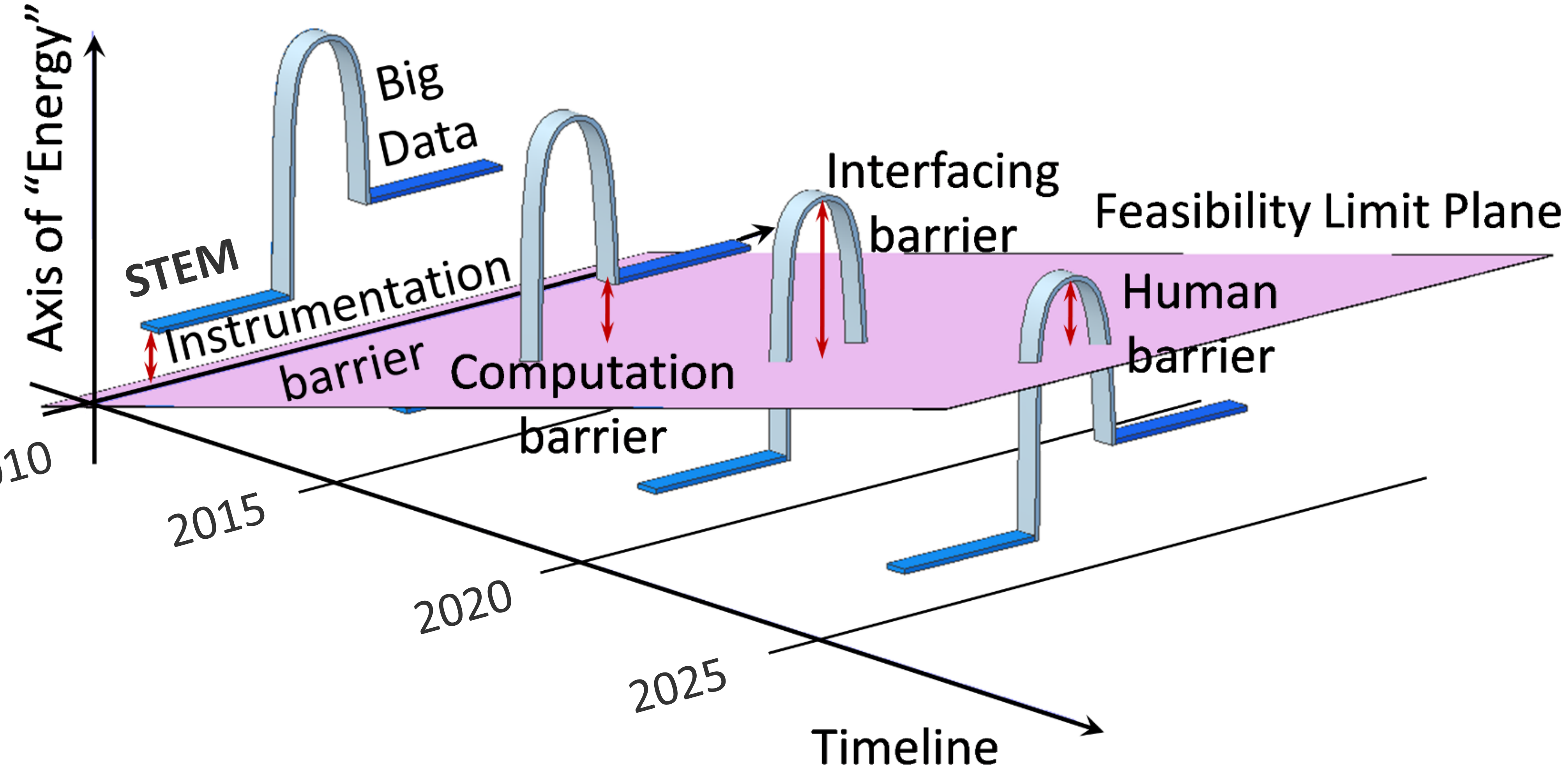
Deep learning in mesoscopic imaging

Model trained on a single movie frame from the well-ordered phase and applied to the entire movie



Maxim Ziatdinov, Xin Li, Shuai Zhang, Harley Pyles, David Baker, James J. De Yoreo, Sergei V. Kalinin

Perspectives



Adapted from figure by S. Jesse