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Variational Autoencoders- III
Applications to Real World Systems

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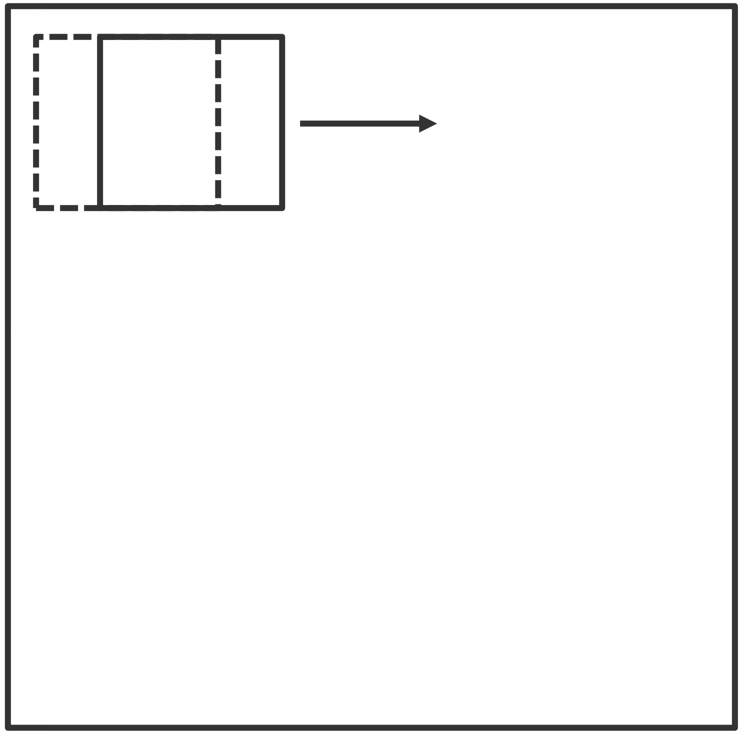
PURPOSE

- (Super-brief) introduction into Neural Networks
- What are (Variational) autoencoders?
- Key notions:
  - Encoding and decoding
  - Latent distribution
  - Latent representations
- Why invariances: rotational, translational, and scale
- Other colors of VAEs:
  - Semi-supervised
  - Conditional
  - Joint
- Real world VAE applications
- From VAEs to encoder-decoders (VED)
- Further opportunities:
  - Physics constraints
  - Representation learning
- Active learning: DKL

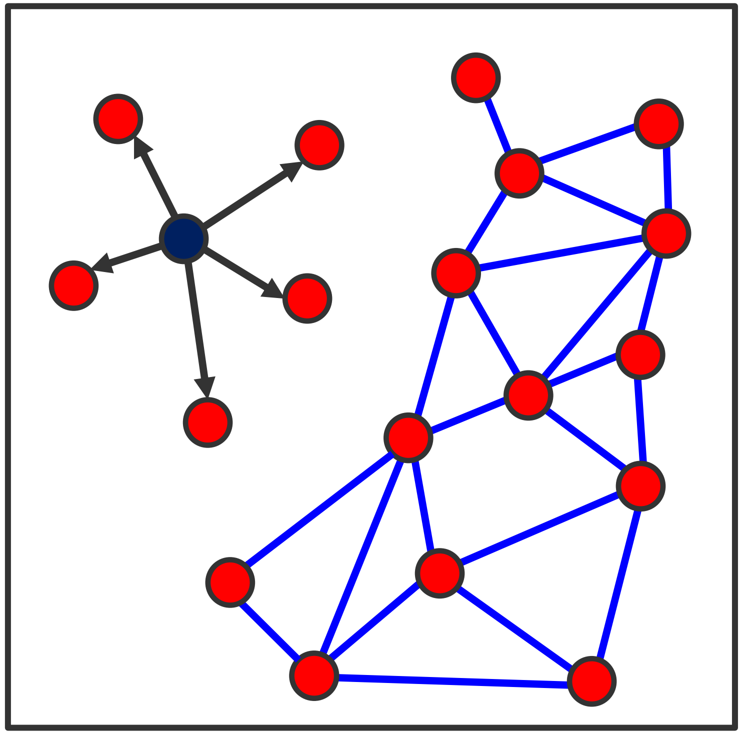
Describing the building blocks

- The classical physical descriptions (symmetry, etc) can be defined locally only in Bayesian sense
- We can argue that local descriptors are simple, if not necessarily known
- And the rules that guide their emergence are also simple, if not known

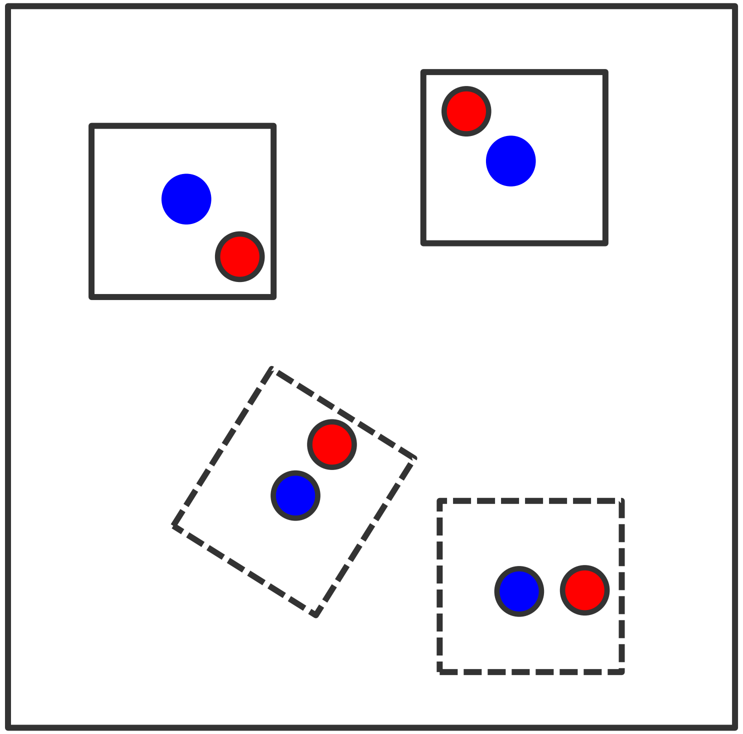
Continuous translational symmetry



Atom based descriptions

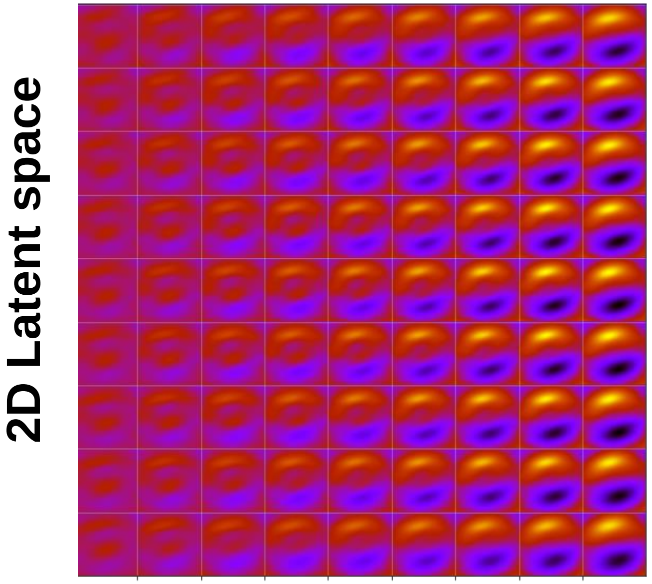


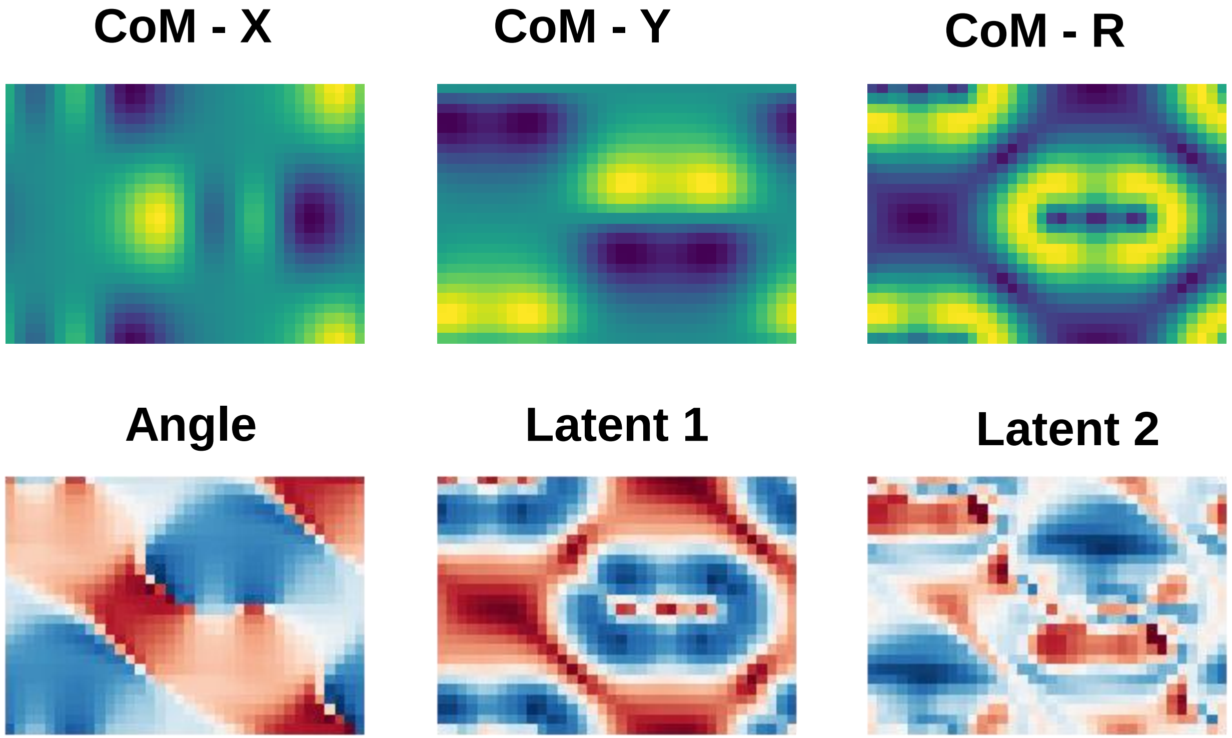
Localized sub-images



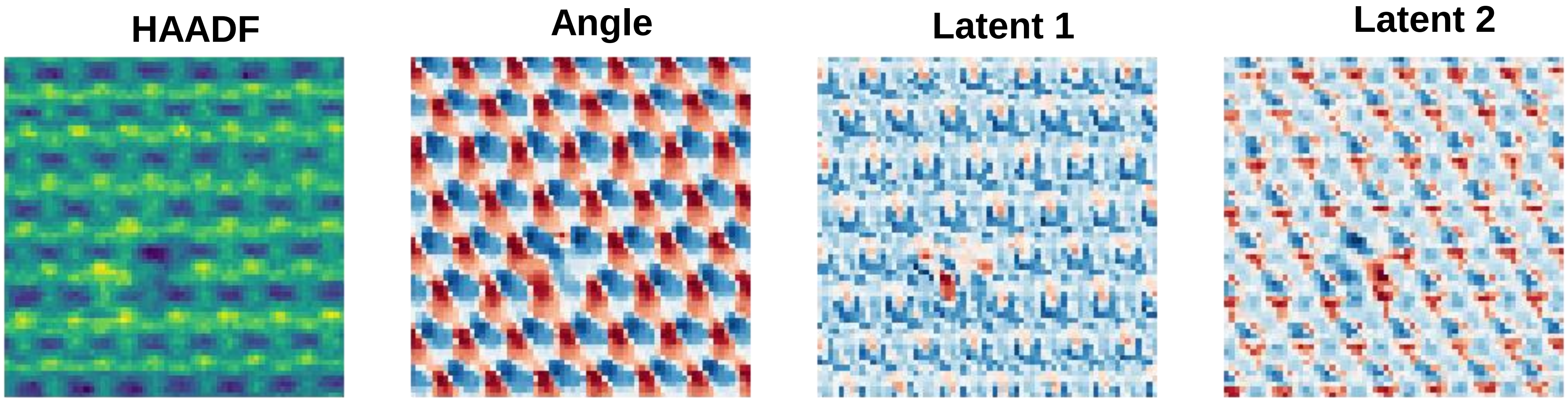
What about 4D STEM?

Simulated 4D STEM for graphene

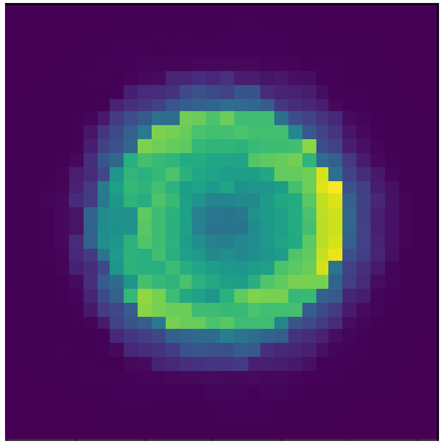


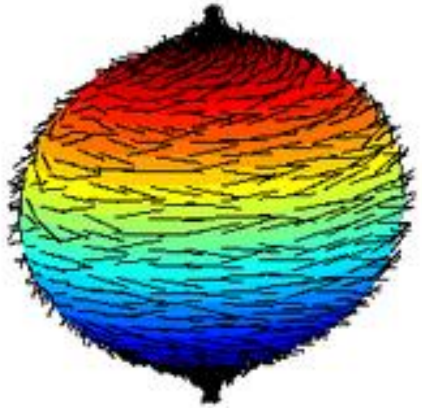


Experiment: vacancy in graphene

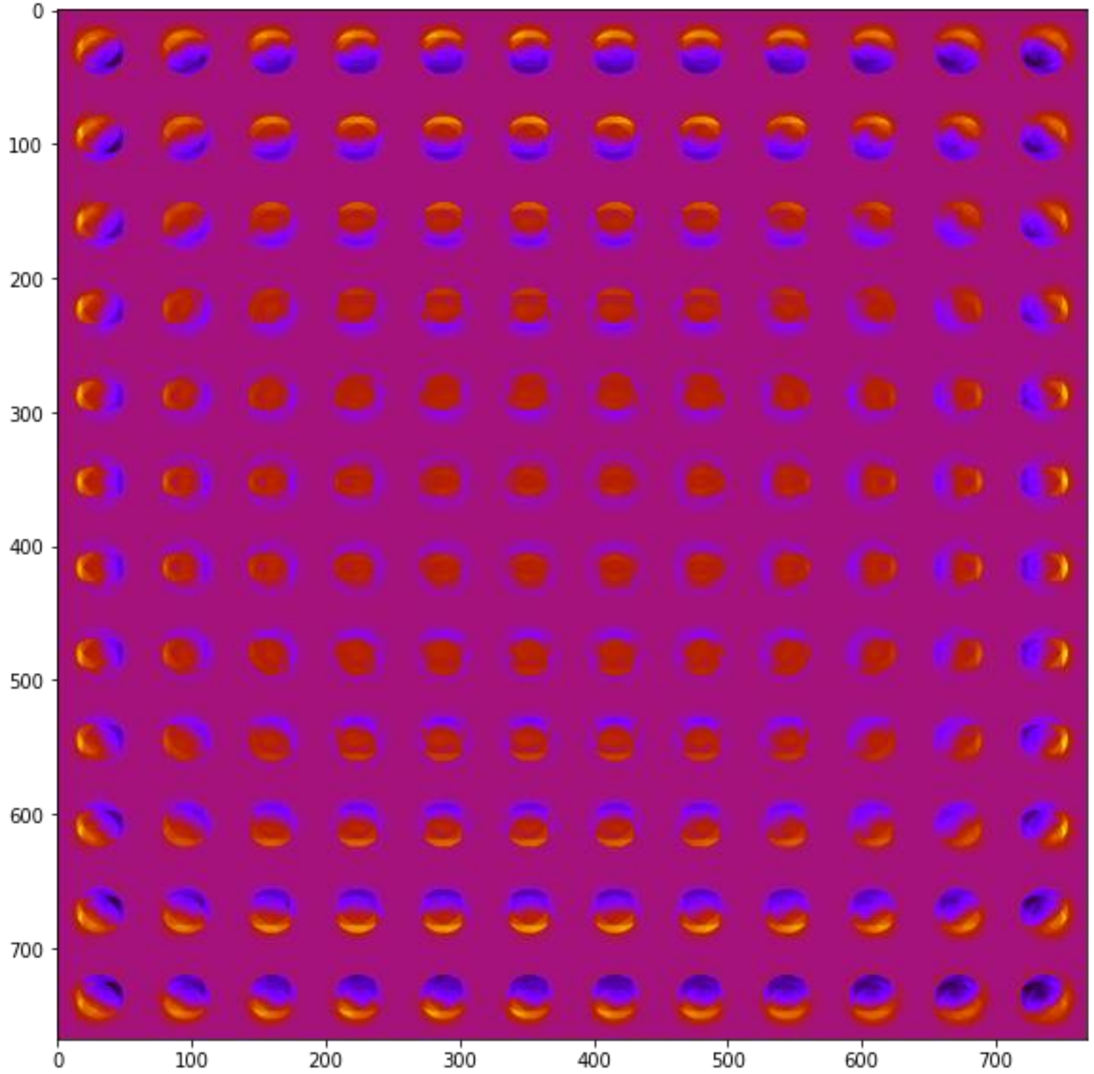


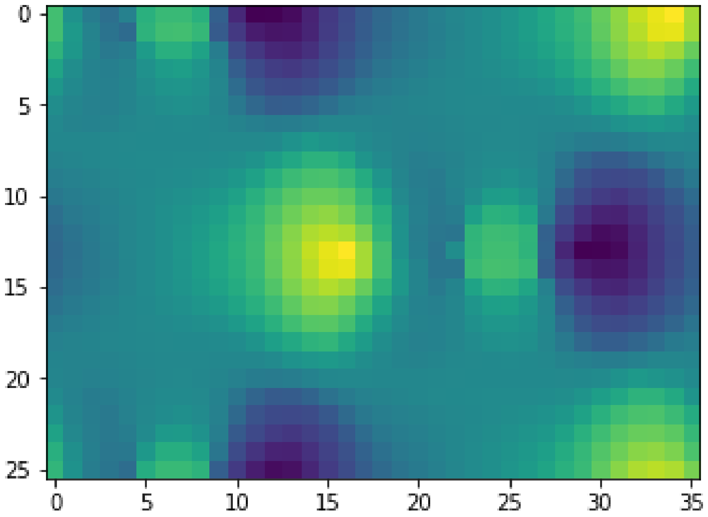
Simple VAE

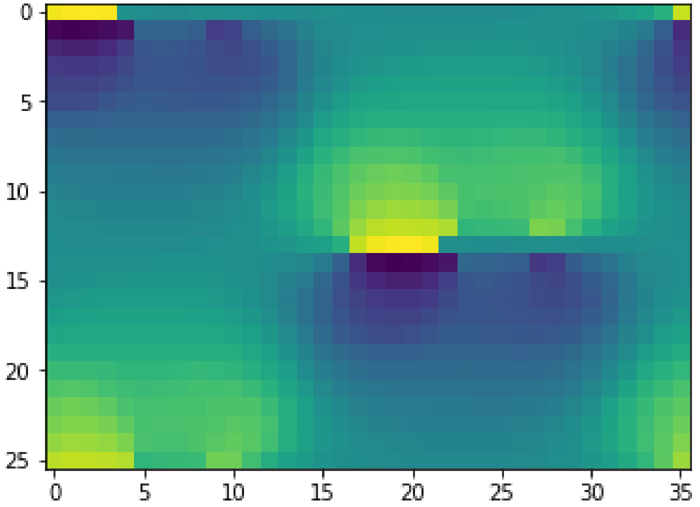




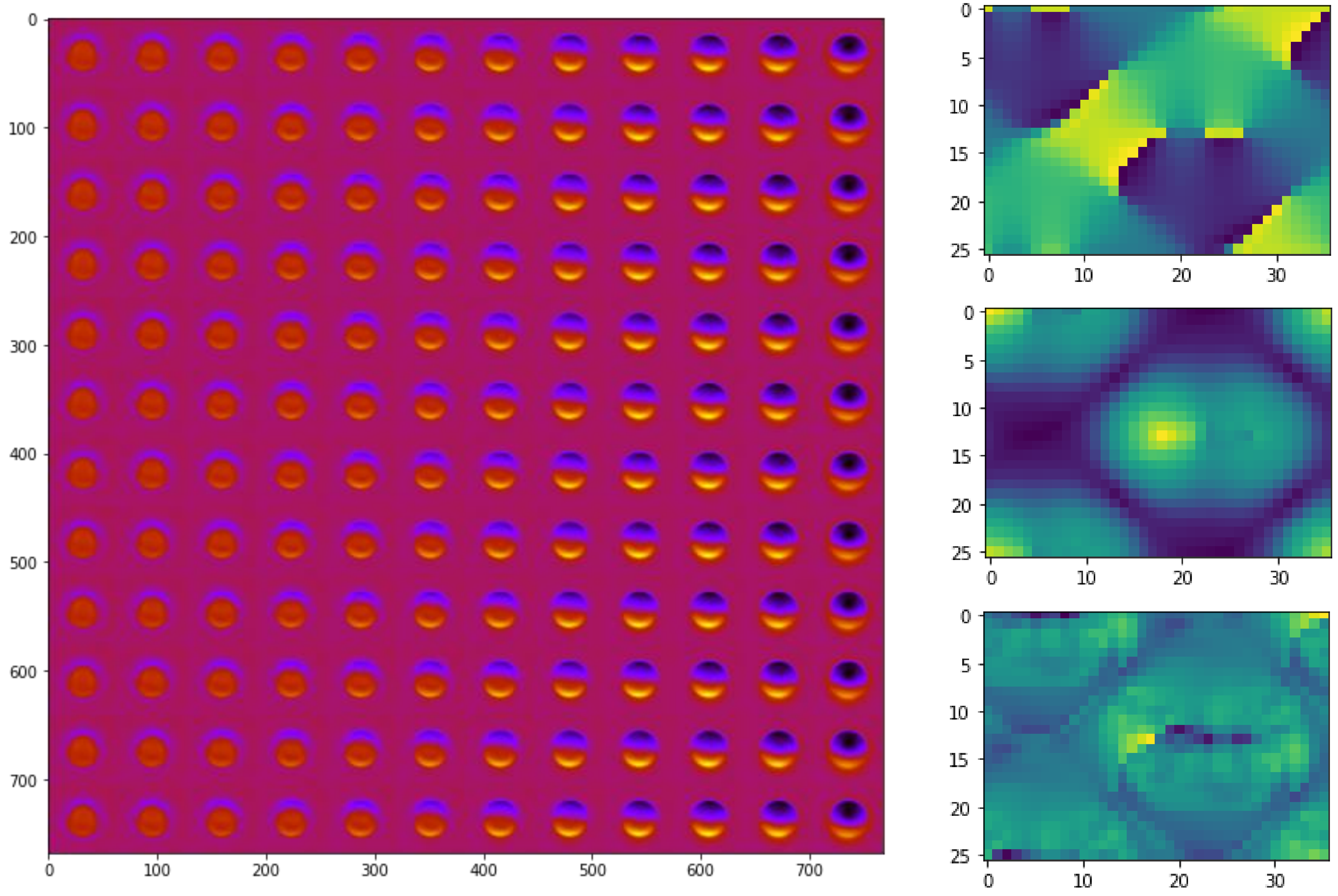
Wikipedia



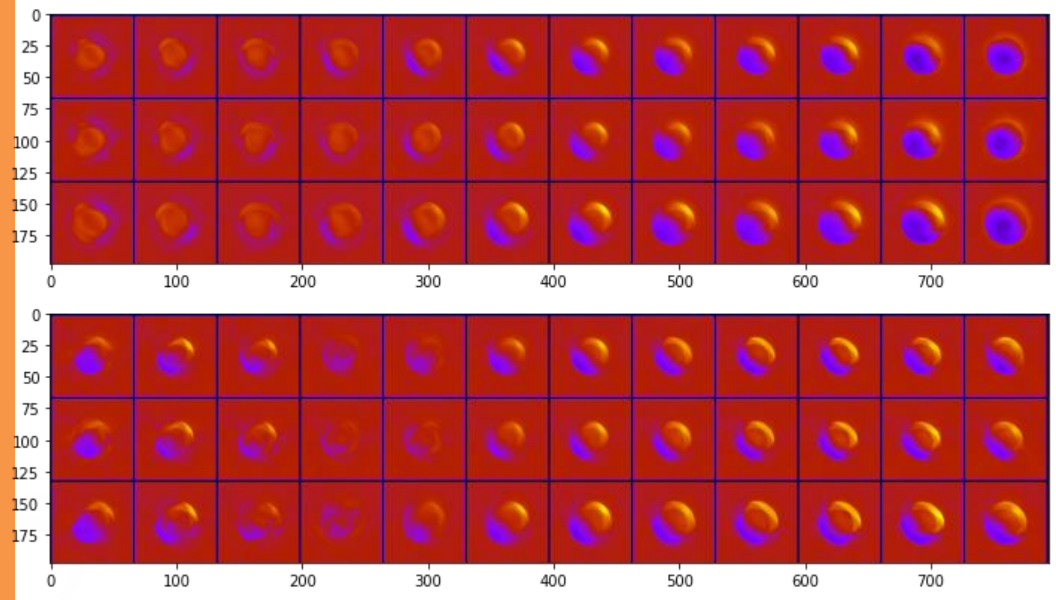


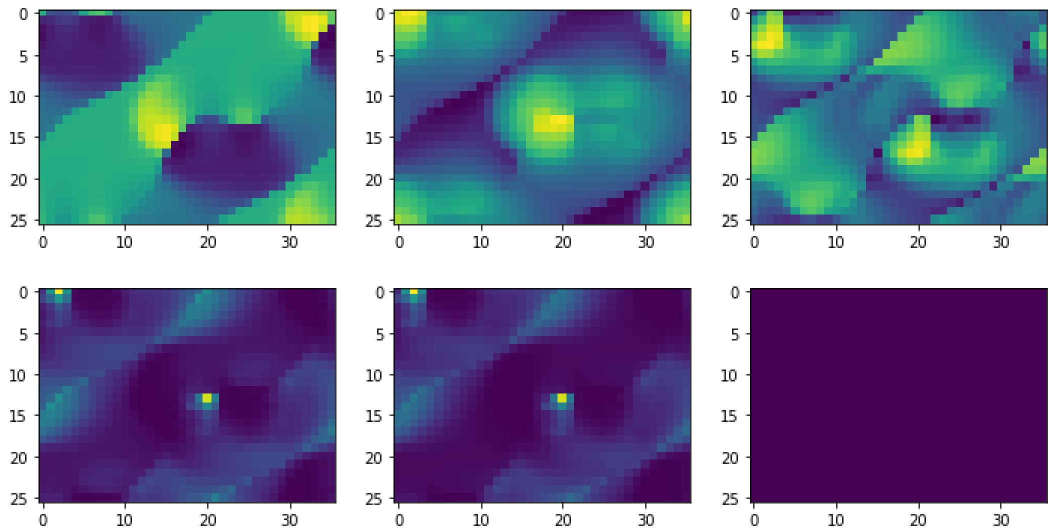


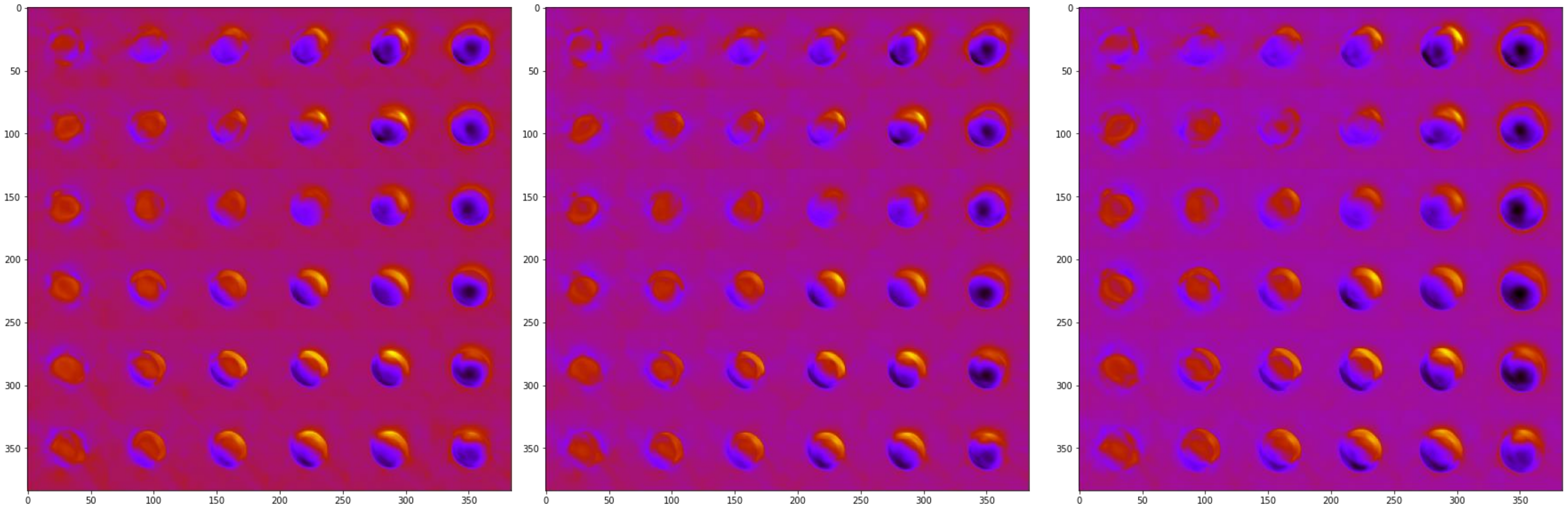
rVAE of 4D STEM



jrVAE of 4D STEM

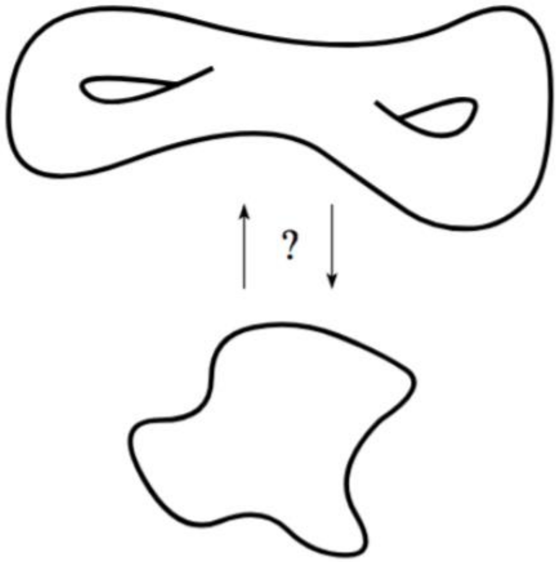


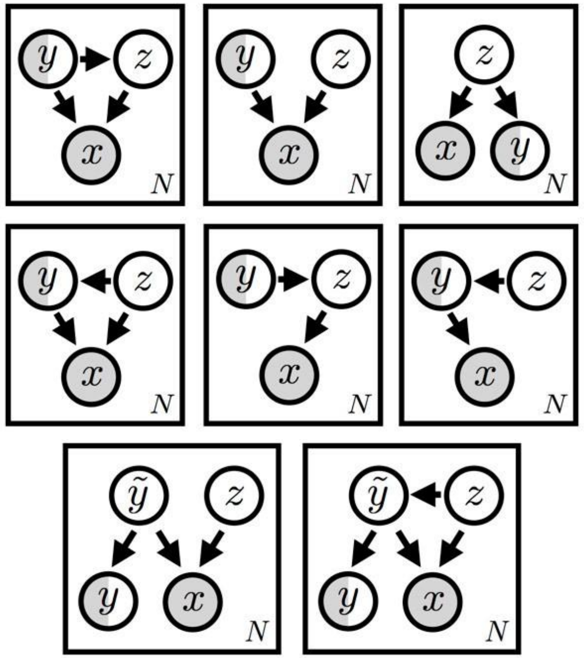




Non-trivial opportunities

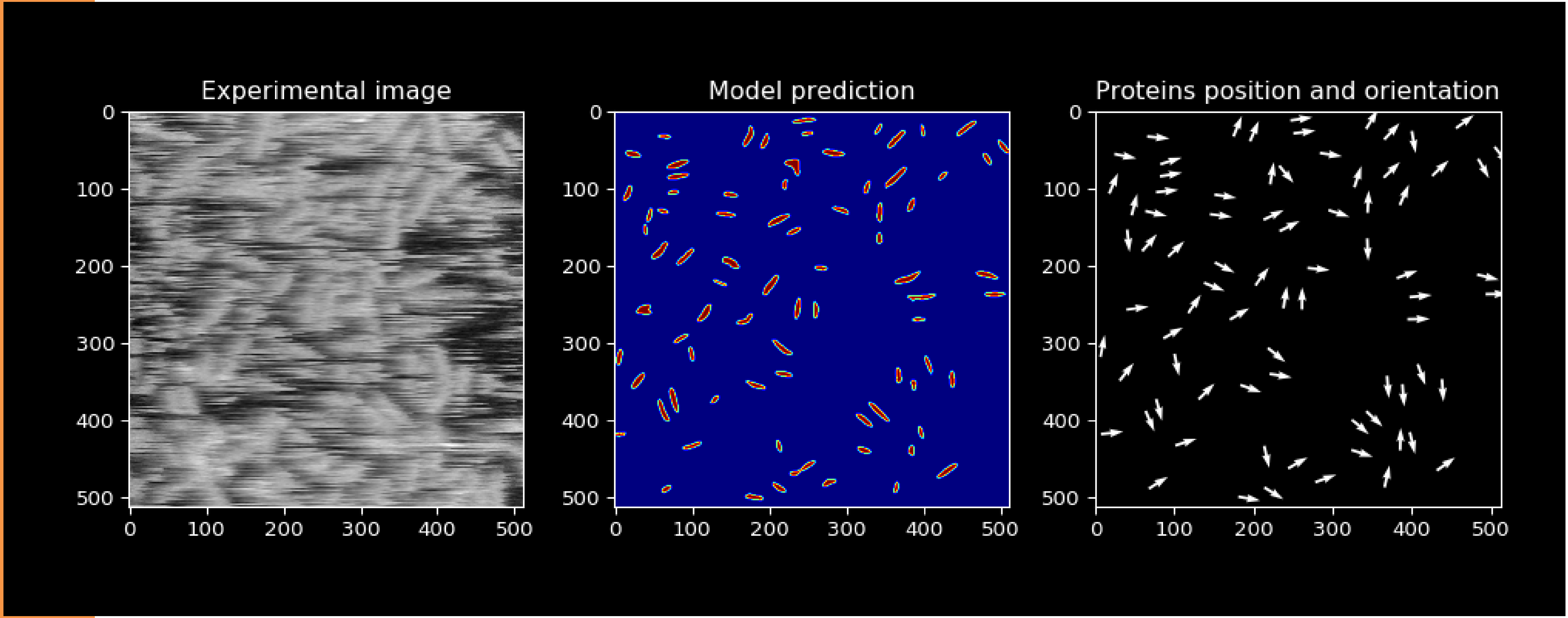
- Extend towards encoder-decoder architectures: structure-property relationships
- Explore adaptation beyond SO(2) group: torus, SO(3), etc.
- Structure DAGs in the latent space
- Applications for scattering?





VAE for ordering nanoparticles

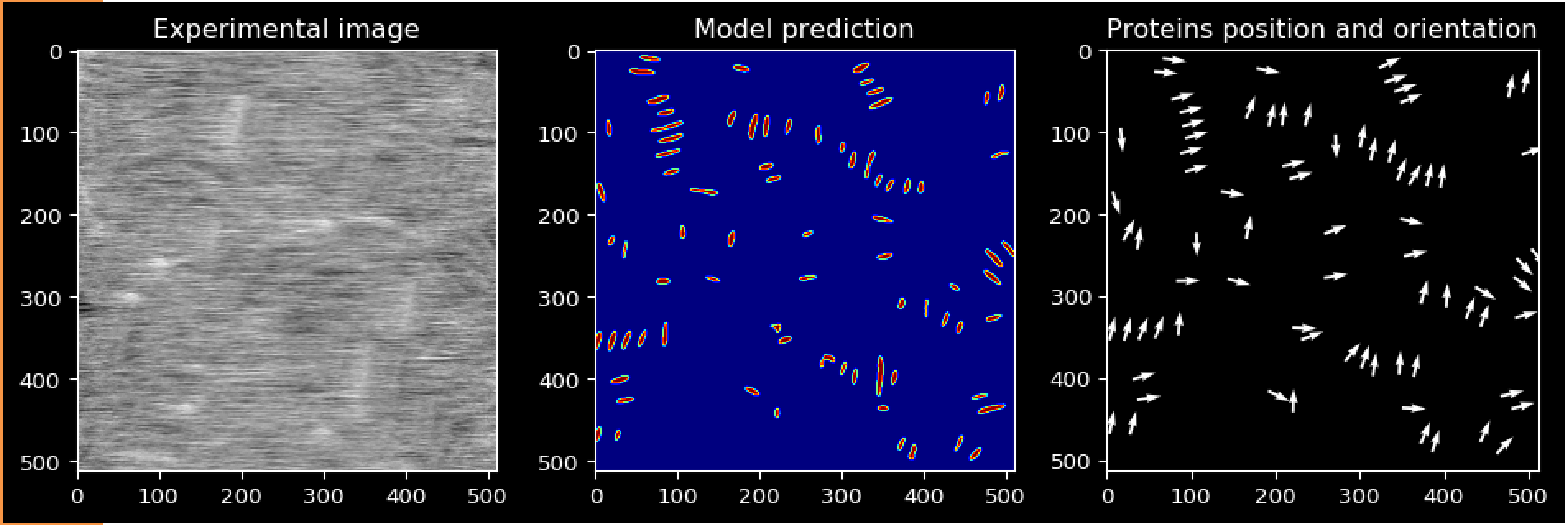
Model trained on a single movie frame from the well-ordered phase and applied to the entire movie



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

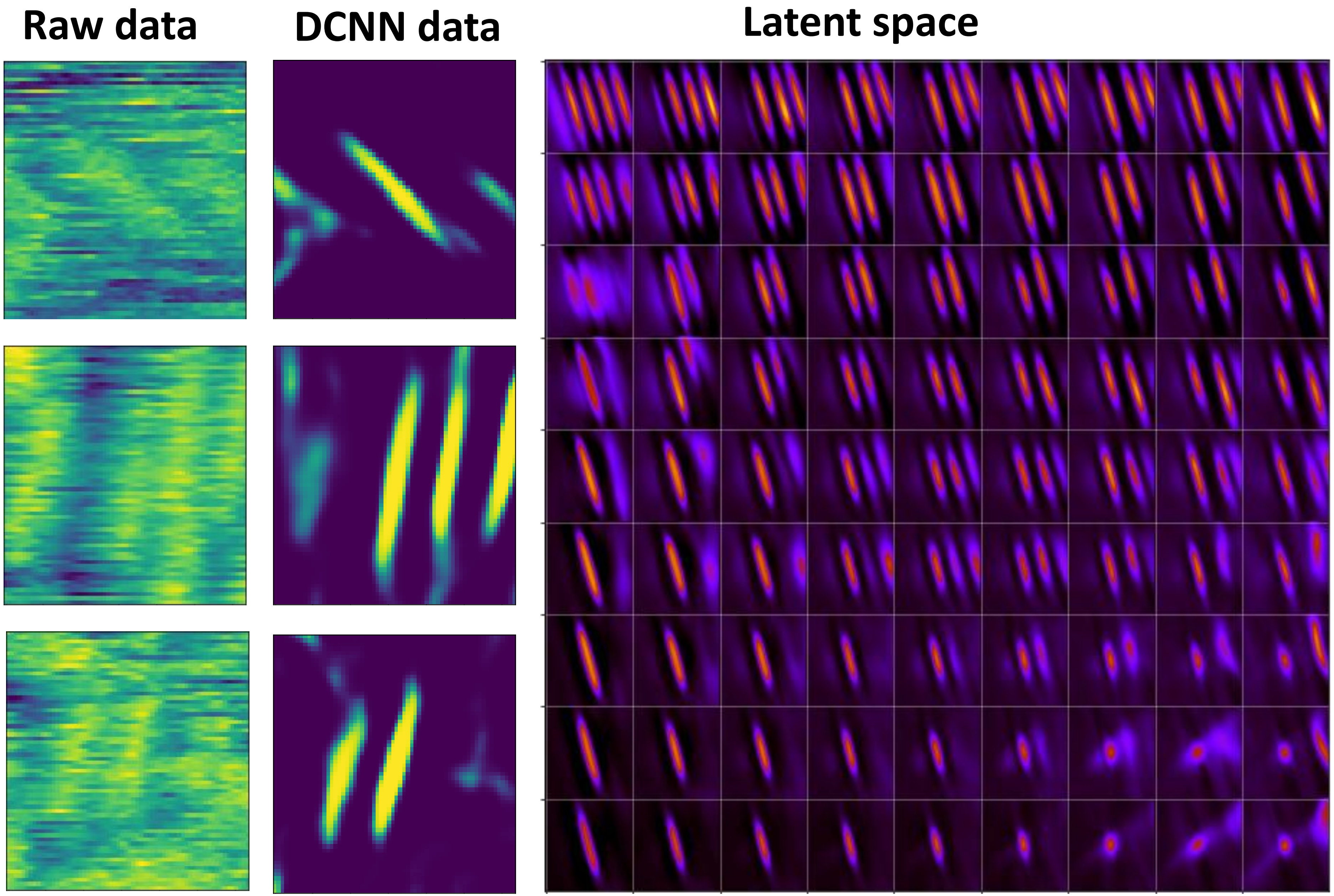
VAE on ordering nanoparticles

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



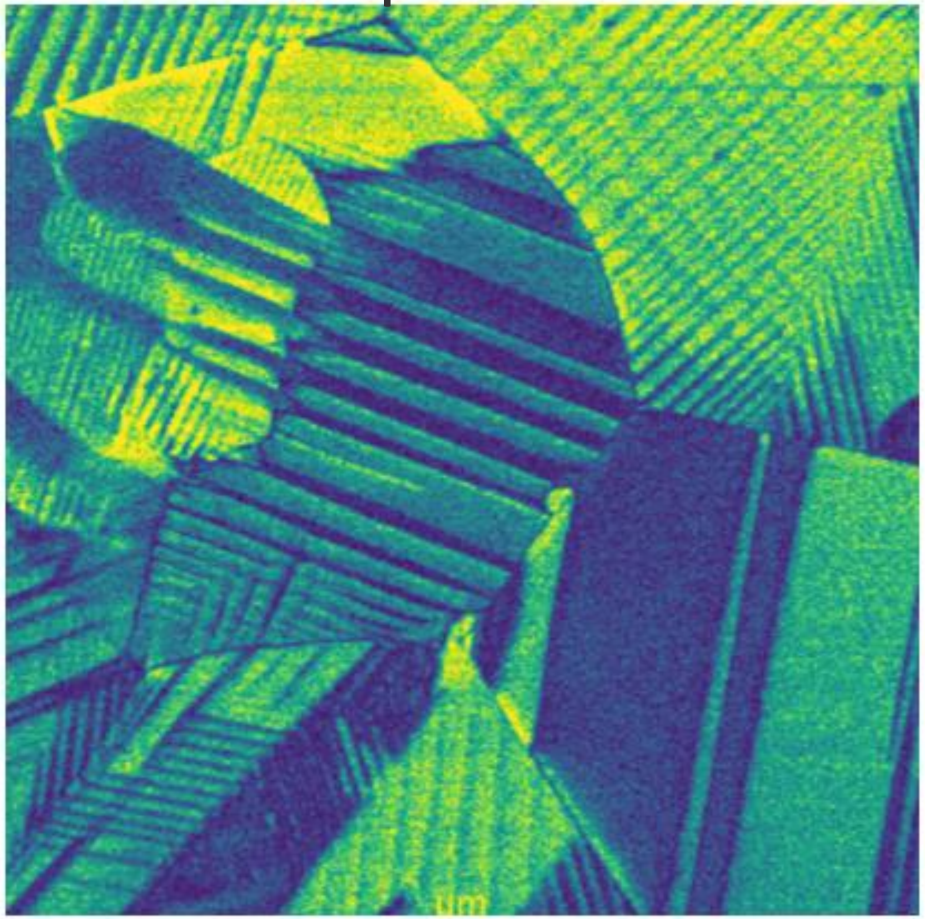
Maxim Ziatdinov, Xin Li, Shuai Zhang, Harley Pyles, David Baker, James J. De Yoreo, Sergei V. Kalinin

Encoding the particles

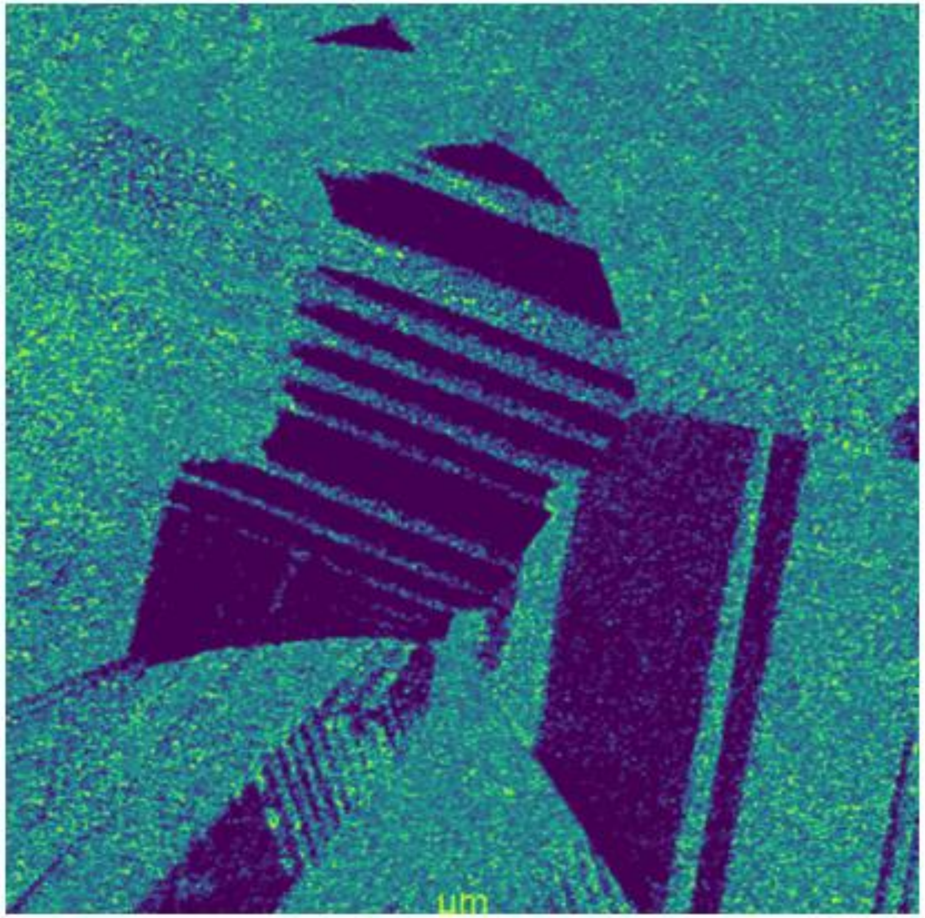


Ferroelectric domain and domain walls

Amplitude

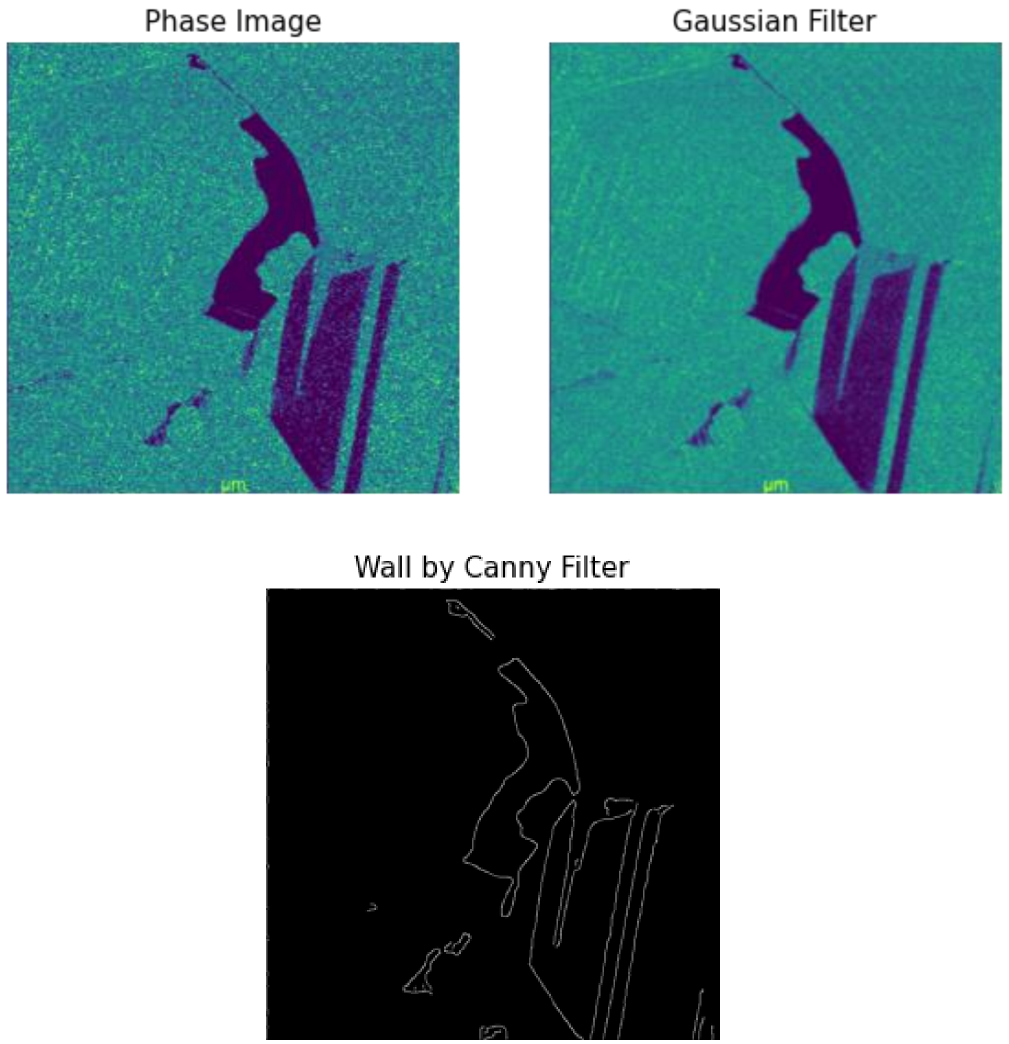


Phase

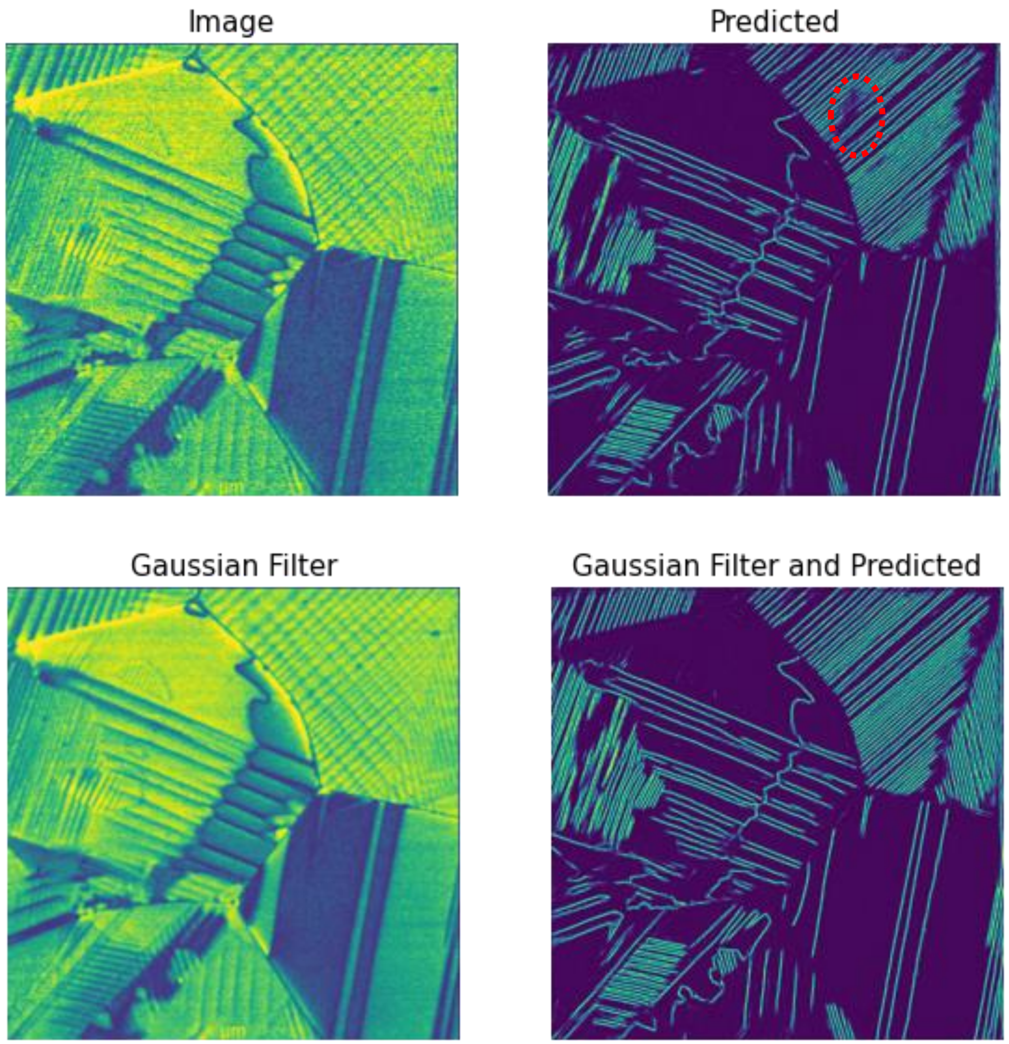


Detecting domain walls

Canny filter

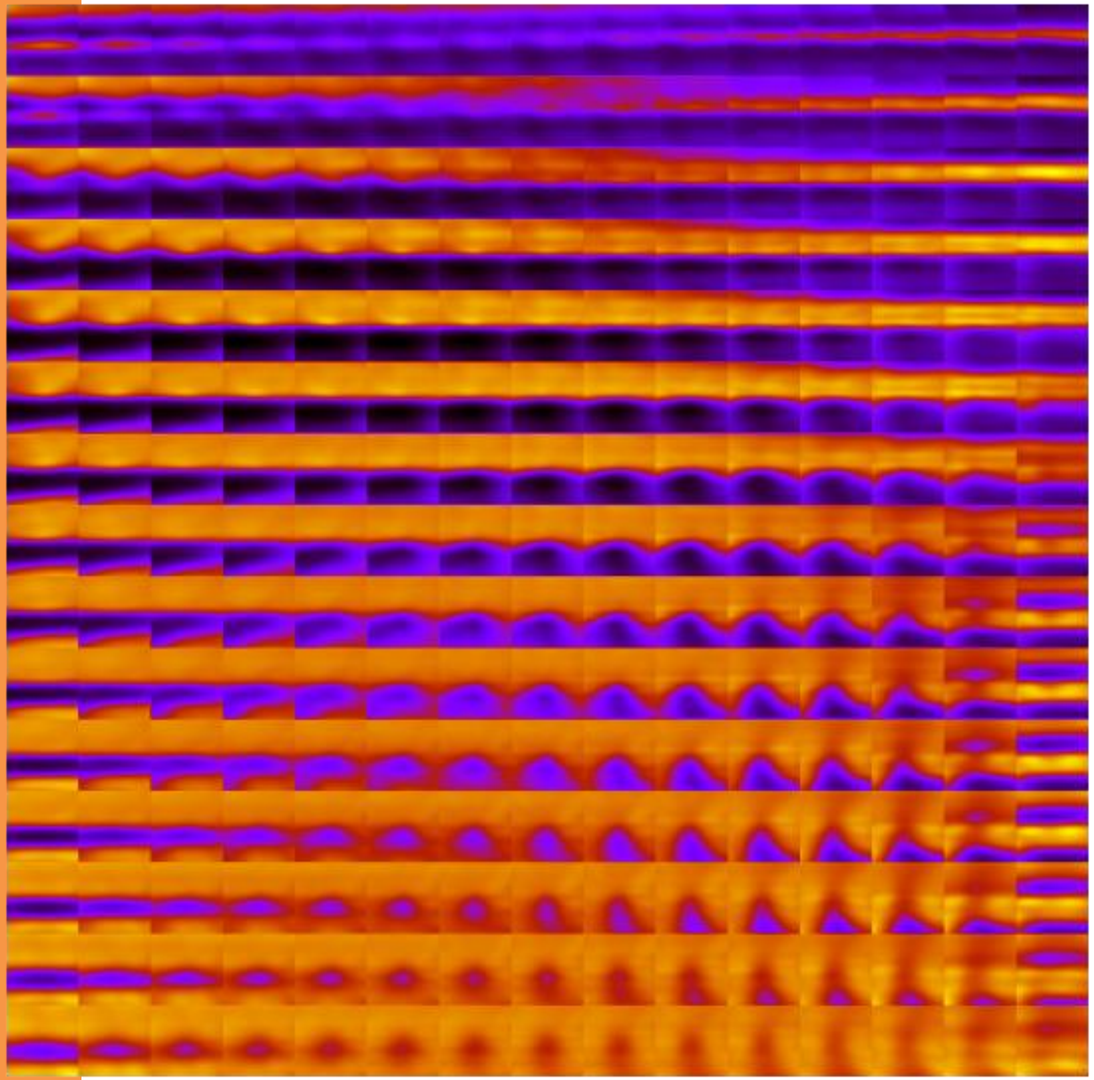


DCNN Prediction

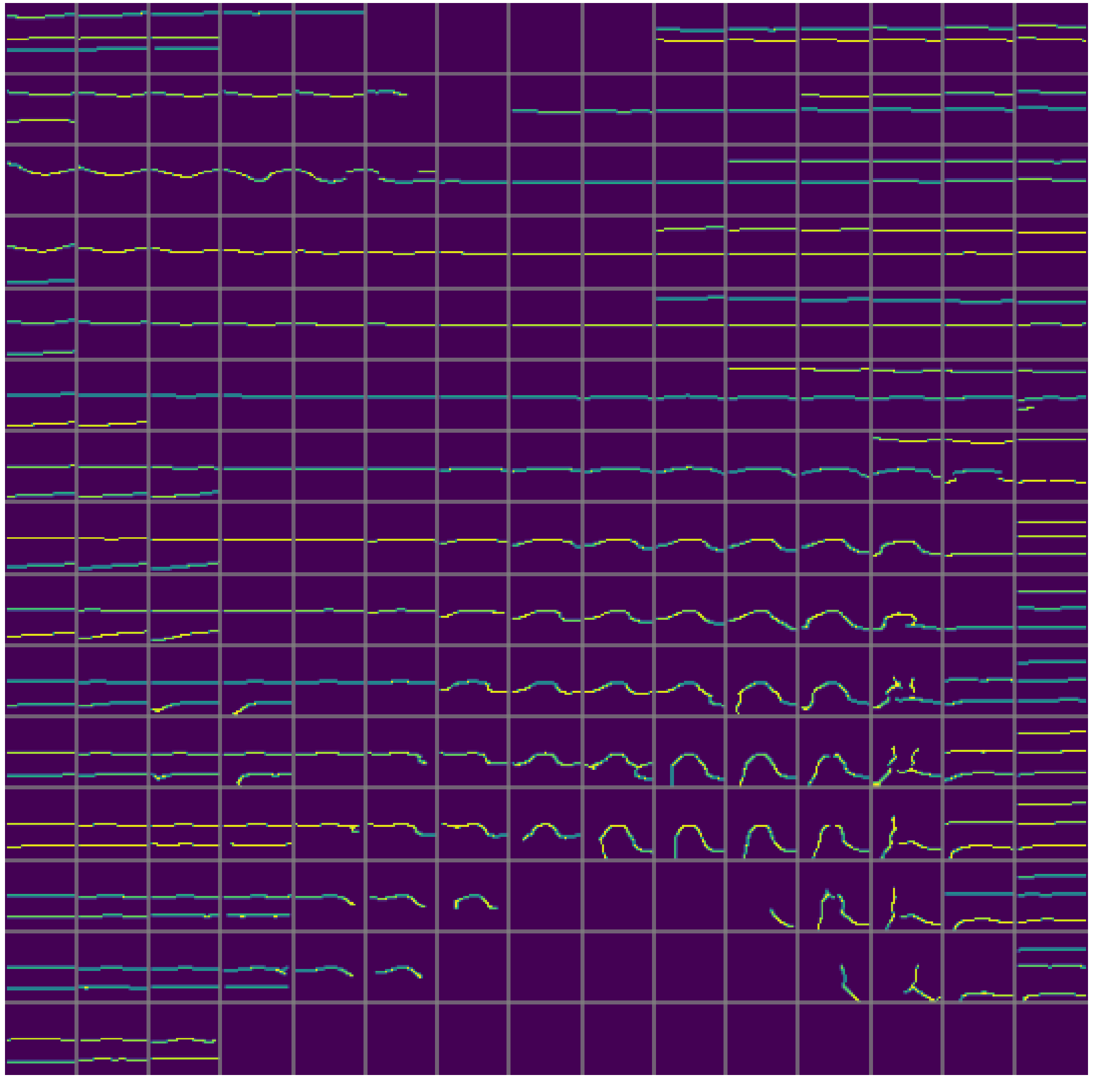


rVAE analysis

Latent Space

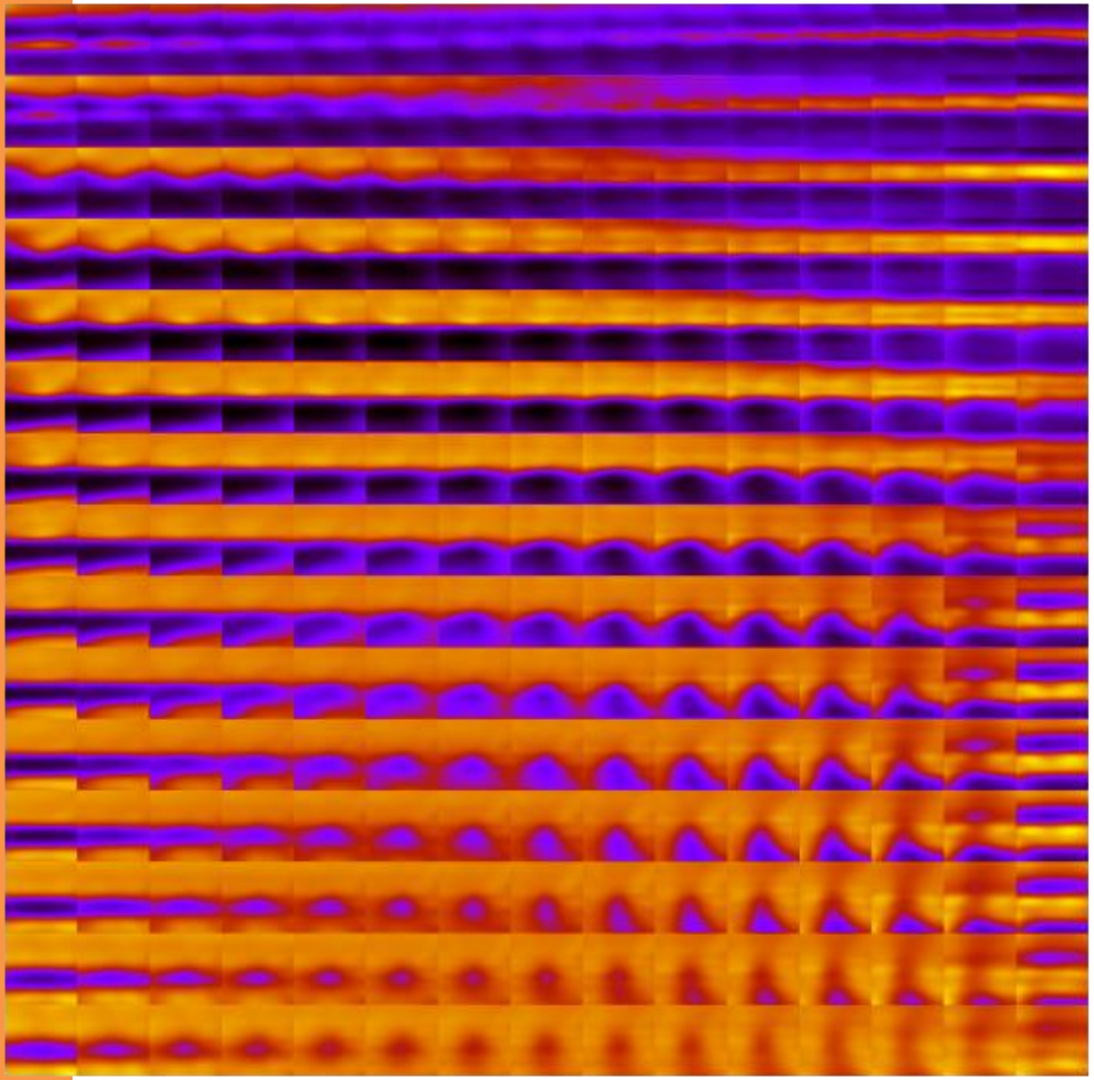


Domain Walls

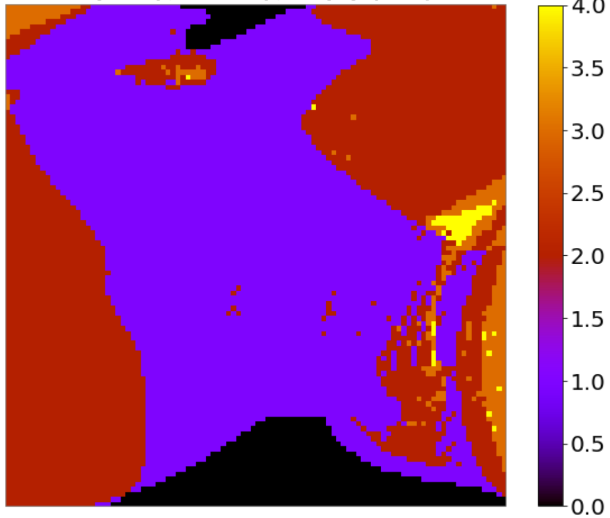


rVAE latent space

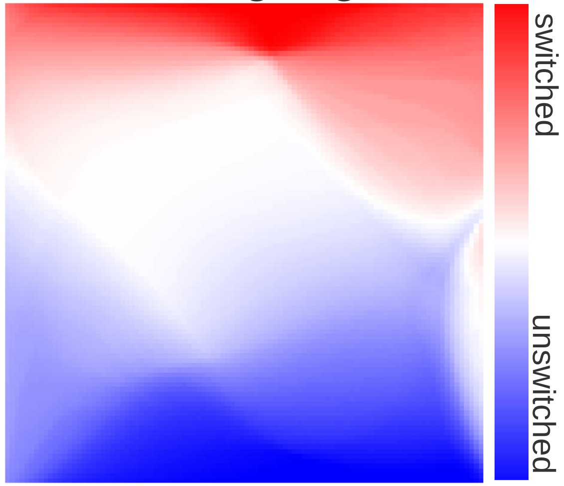
Latent Space



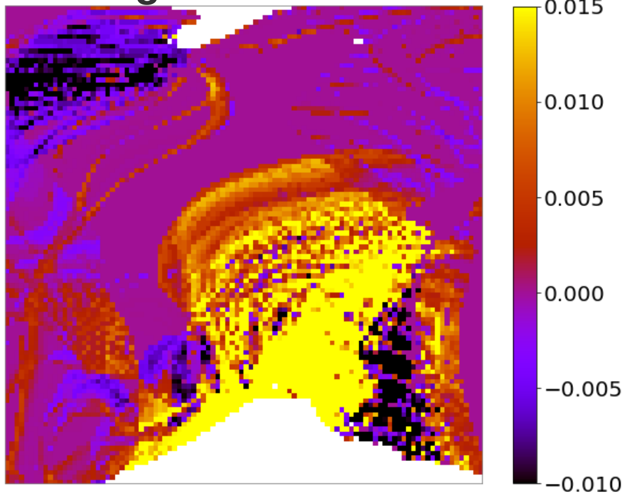
Domain wall count



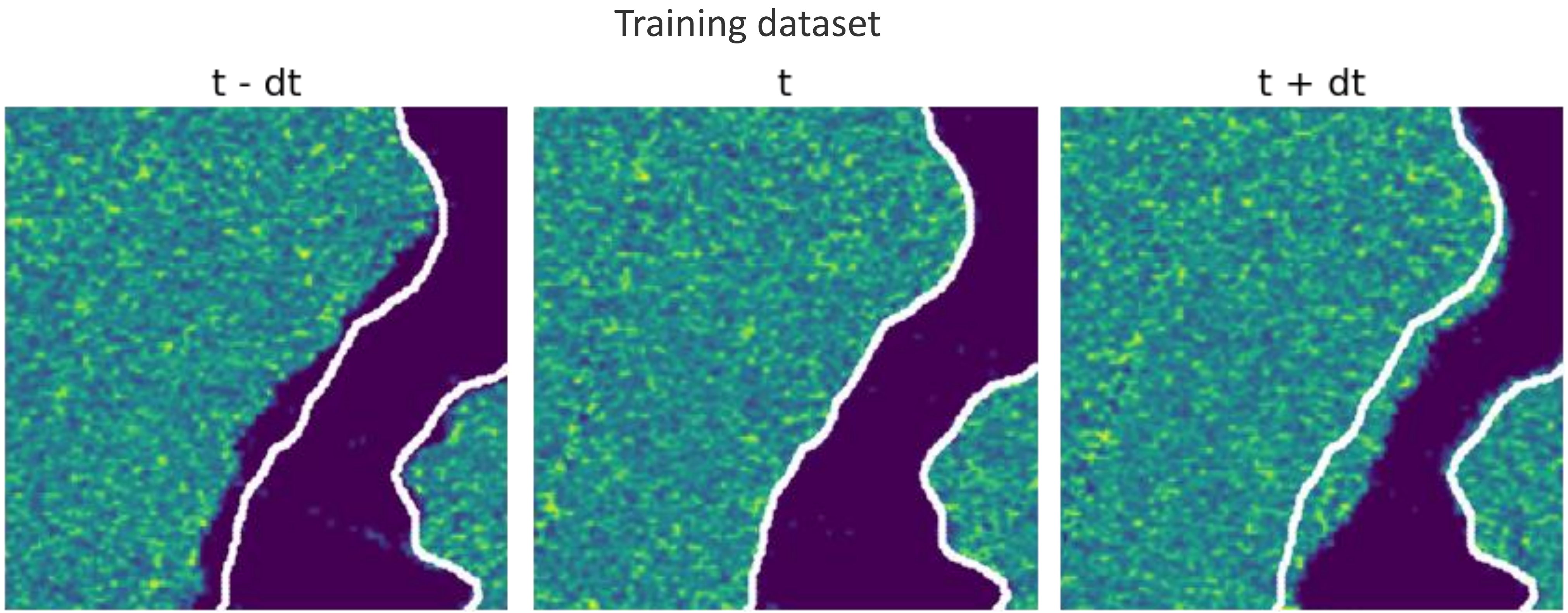
Switching degree



Average wall curvature

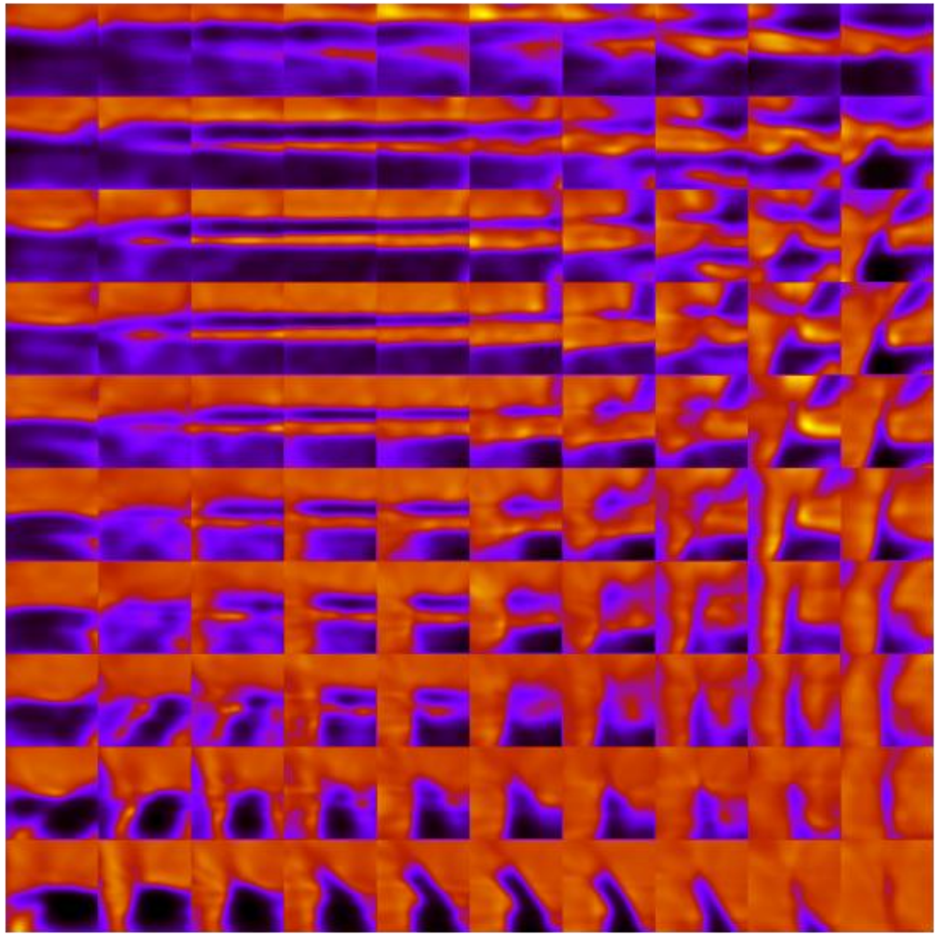


rVAE with time delay

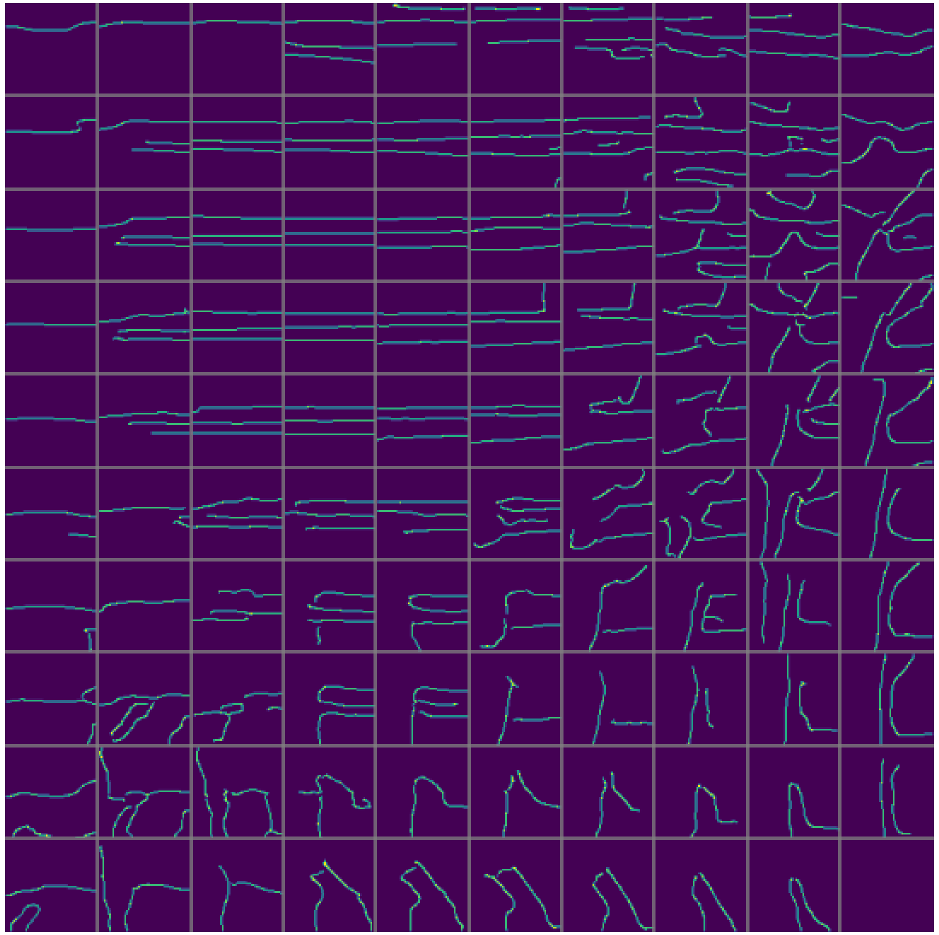


rVAE with time delay

Latent space

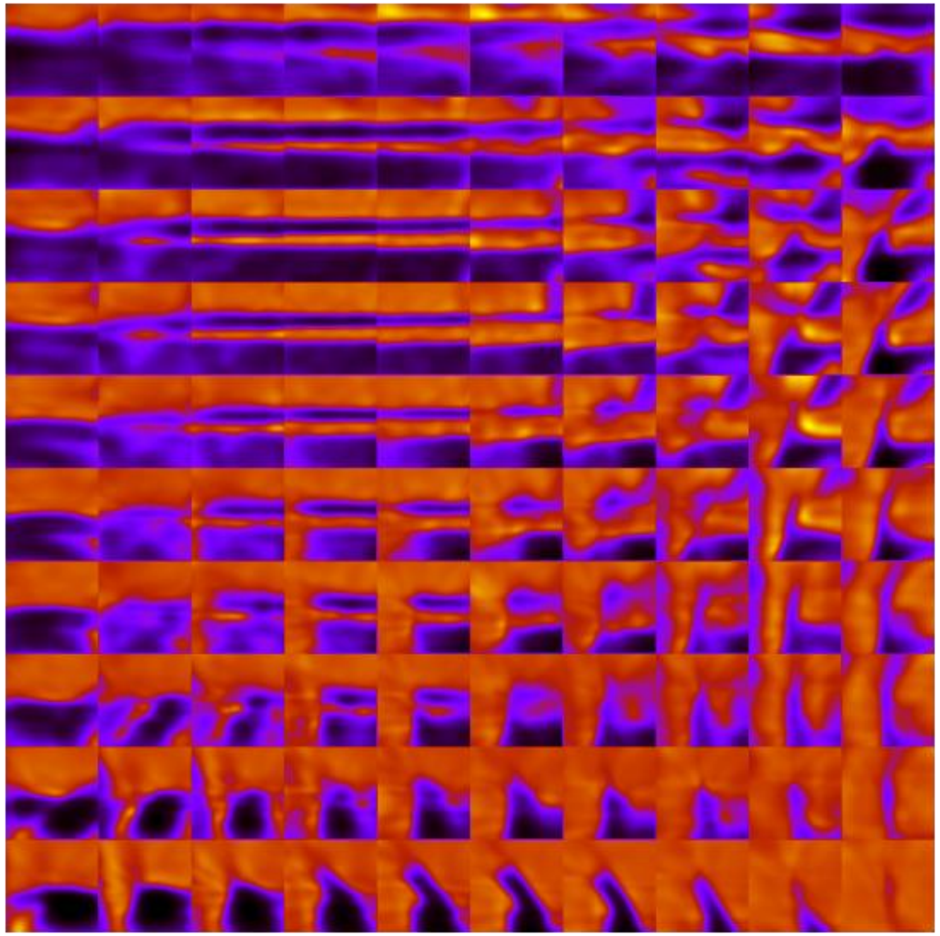


Domain wall

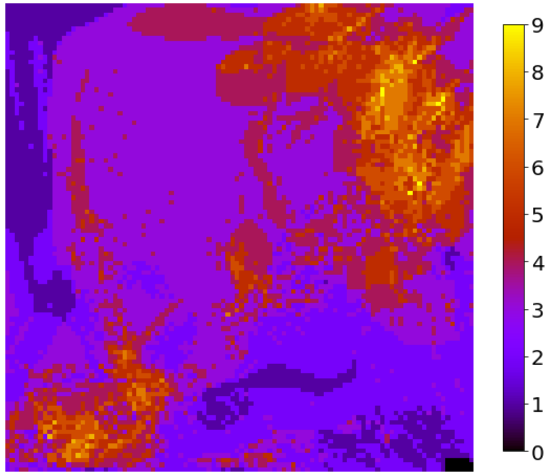


rVAE with time delay

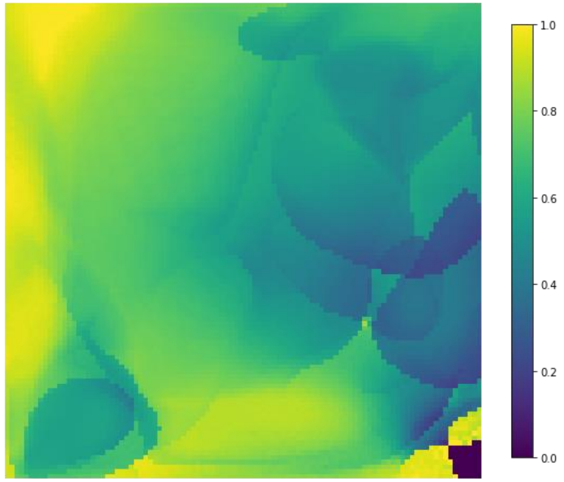
Latent space



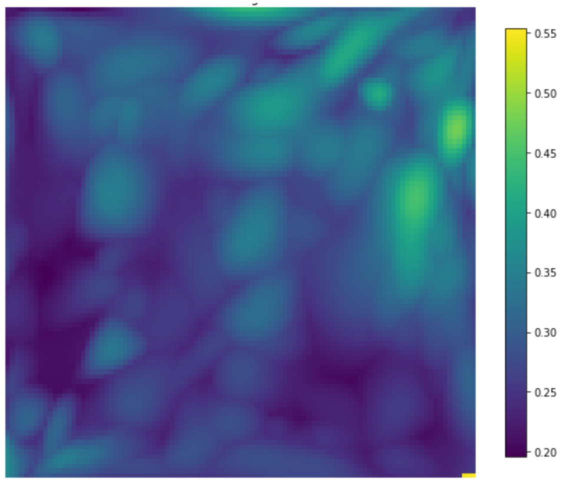
Wall count



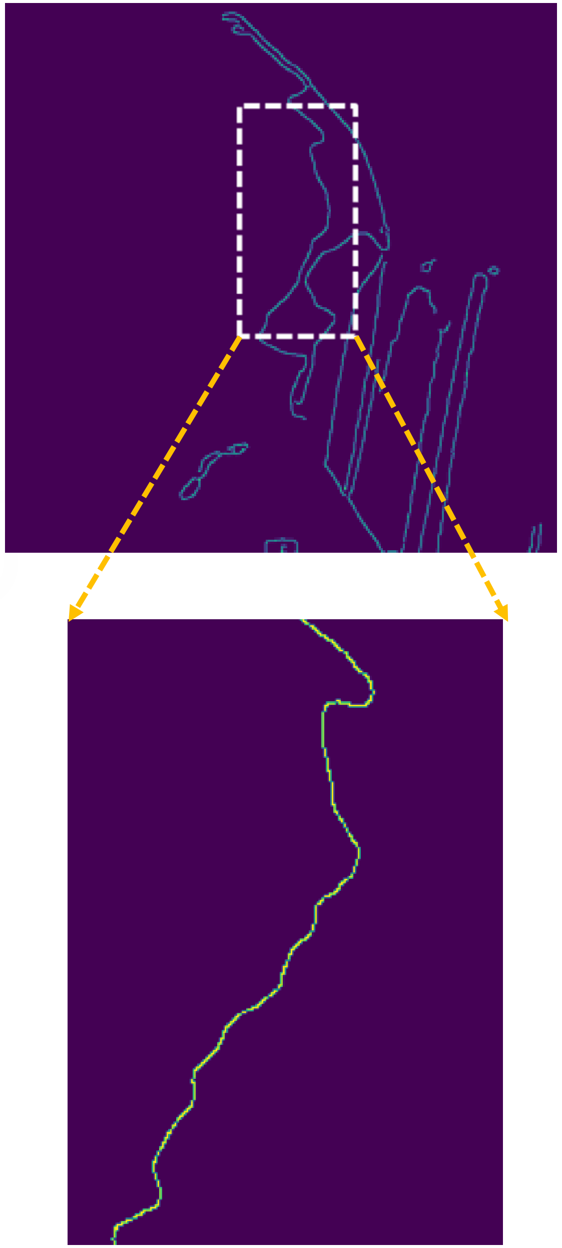
Domain convex

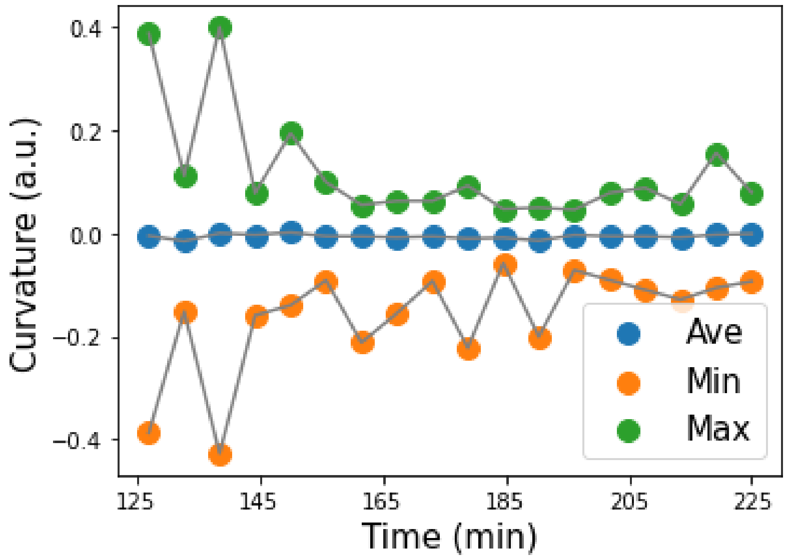


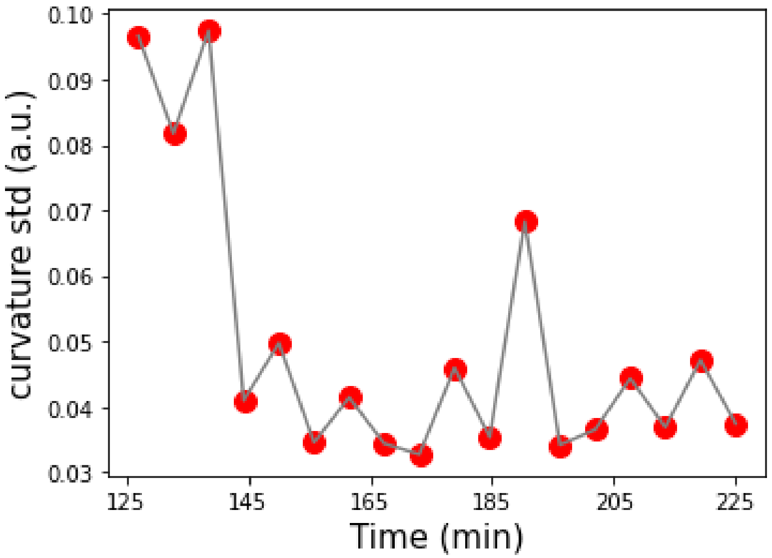
Switch significance



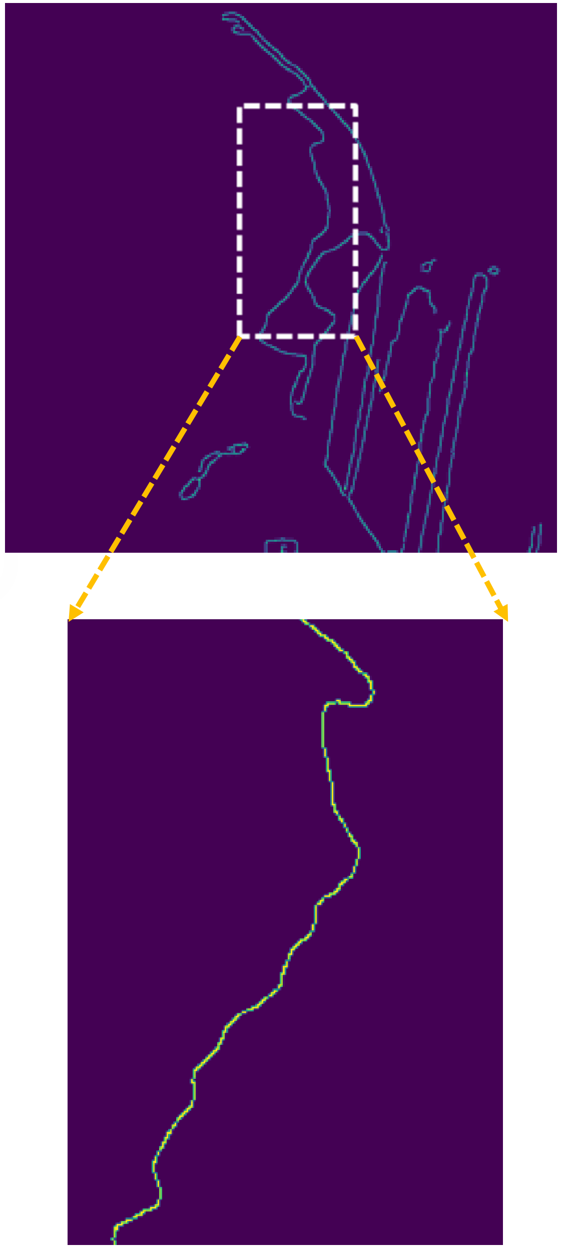
Domain wall evolution





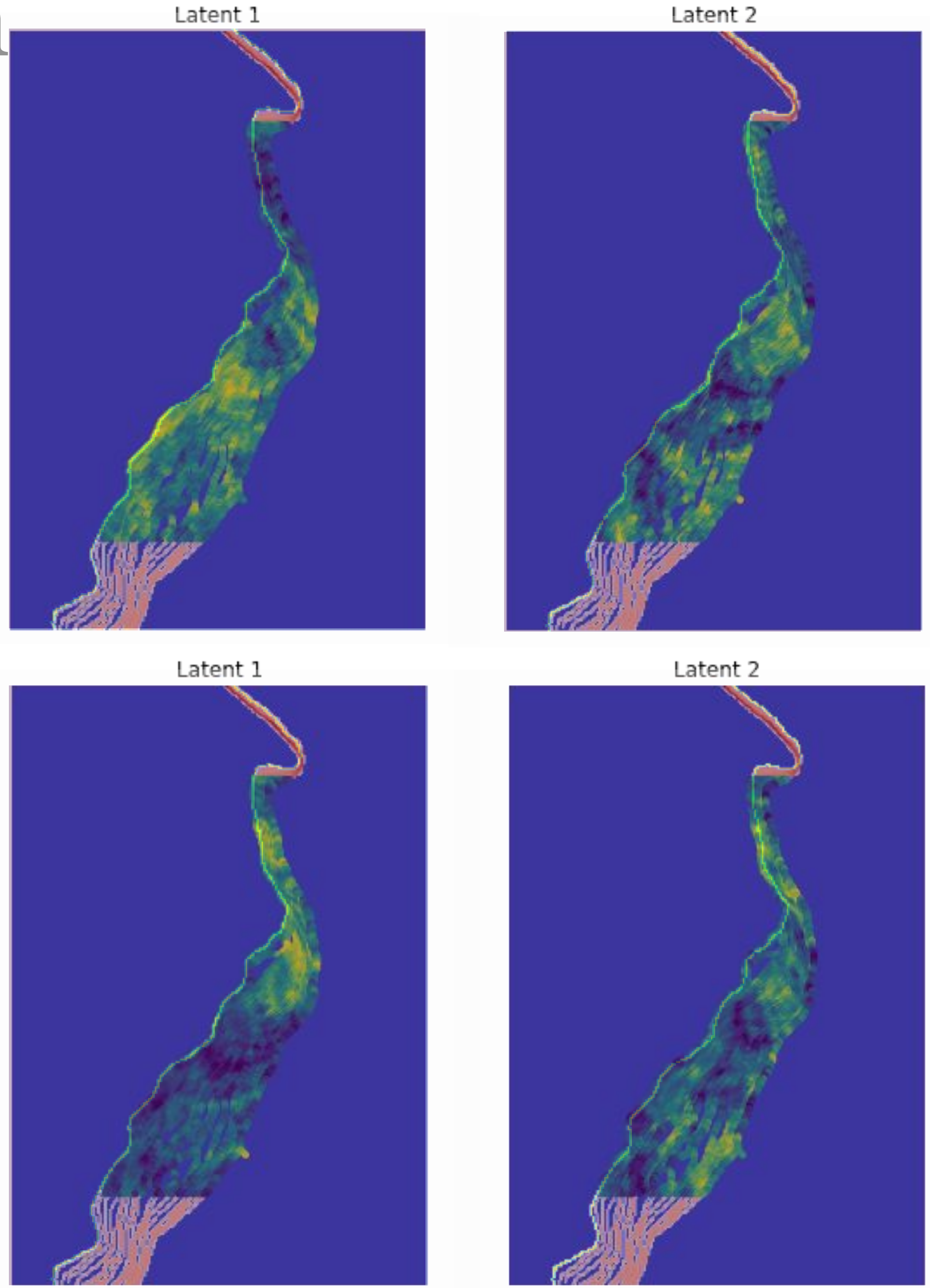


Domain wall evolution

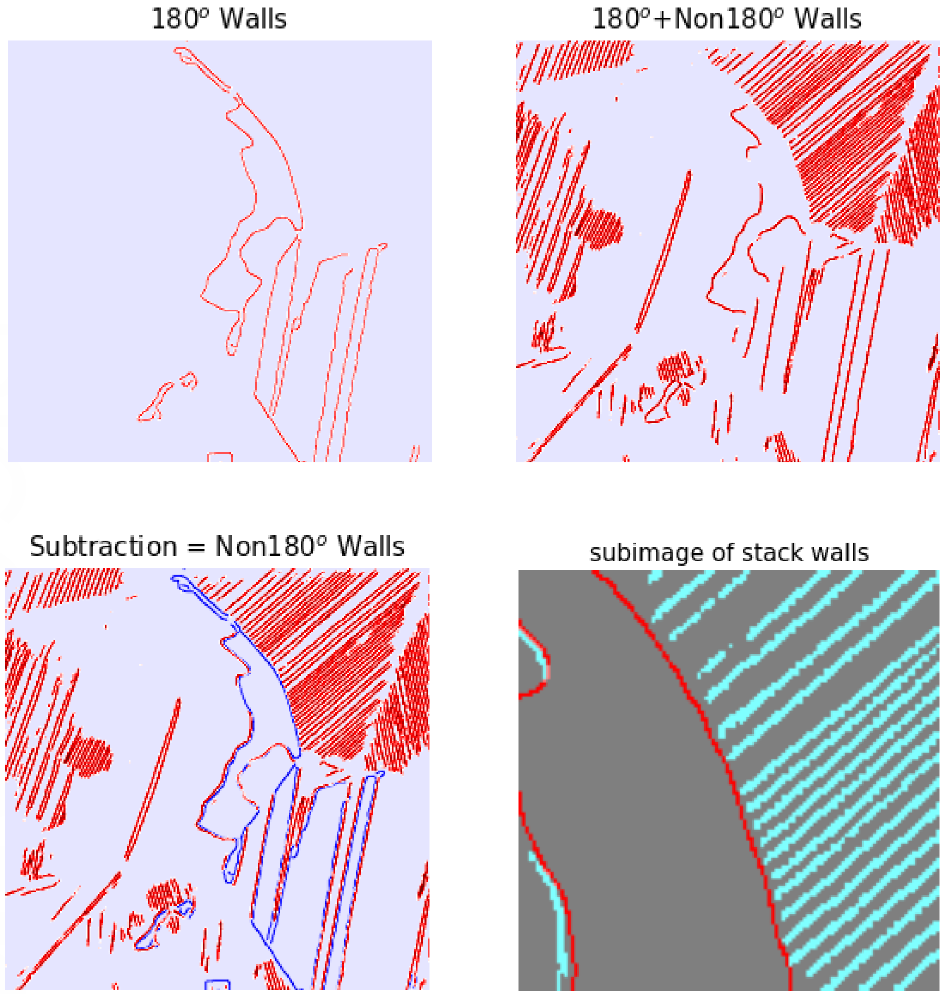


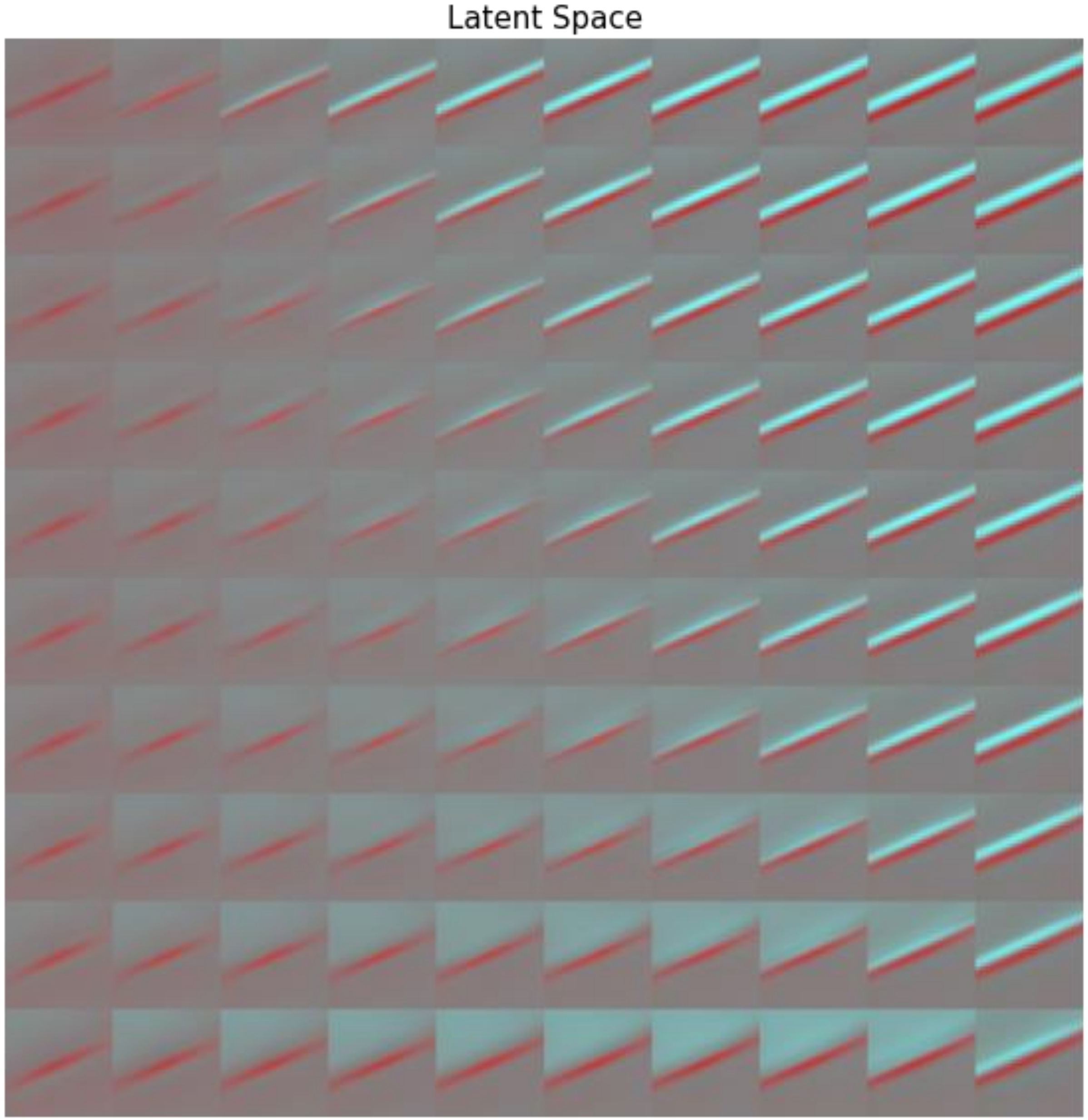
Forward:
t vs t+1

Reverse:
t vs t+1

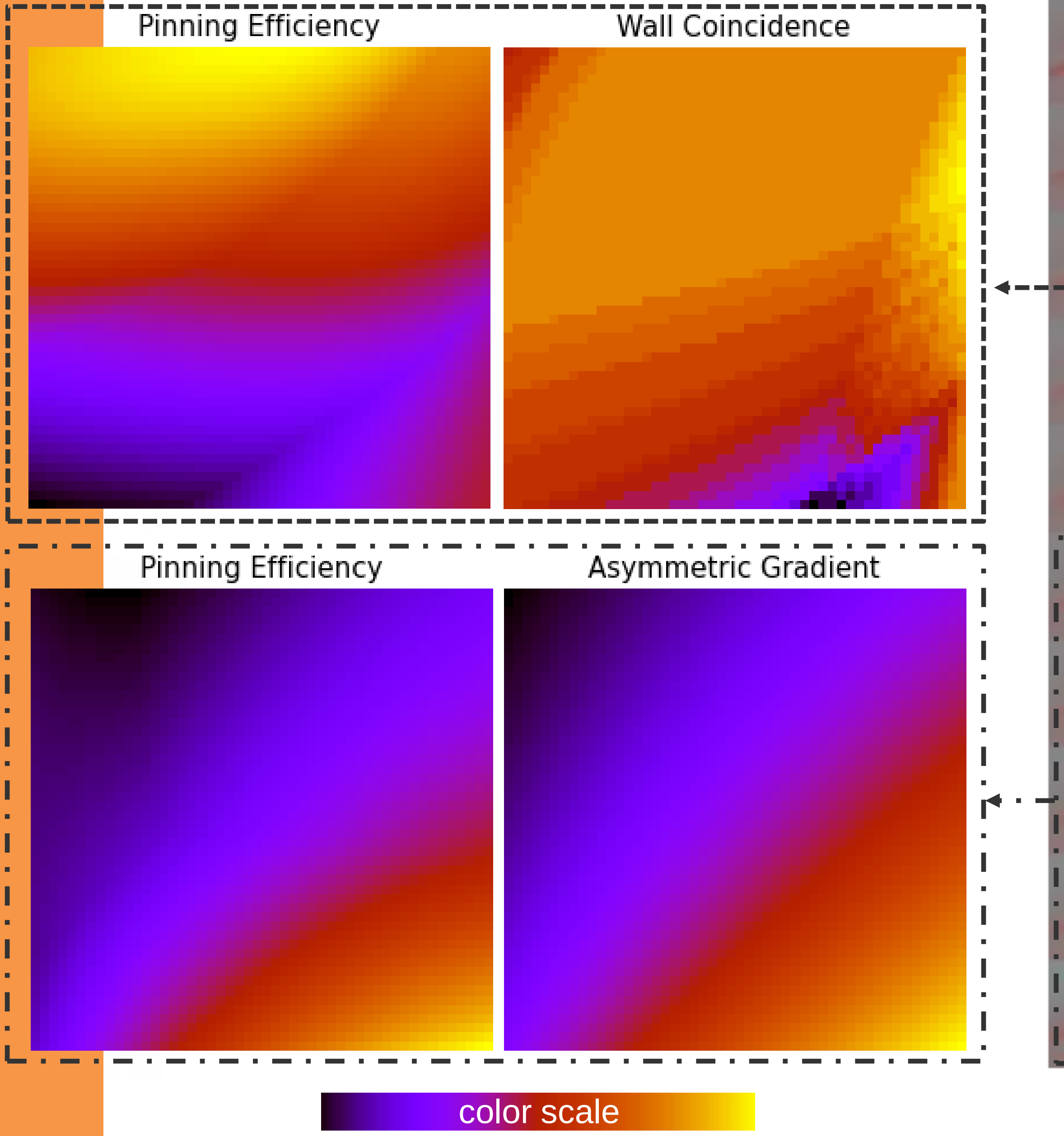


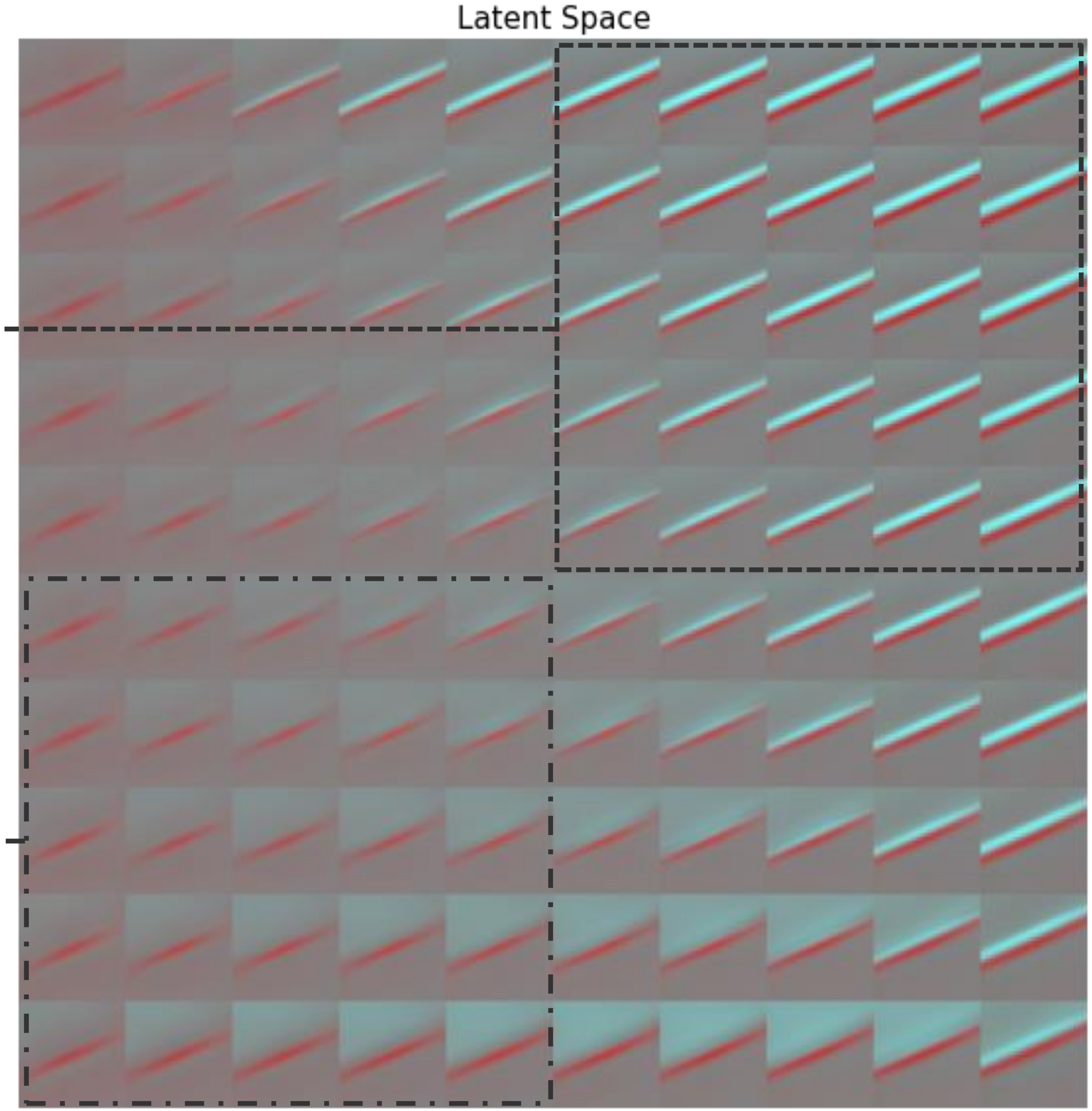
Multilayer rVAE



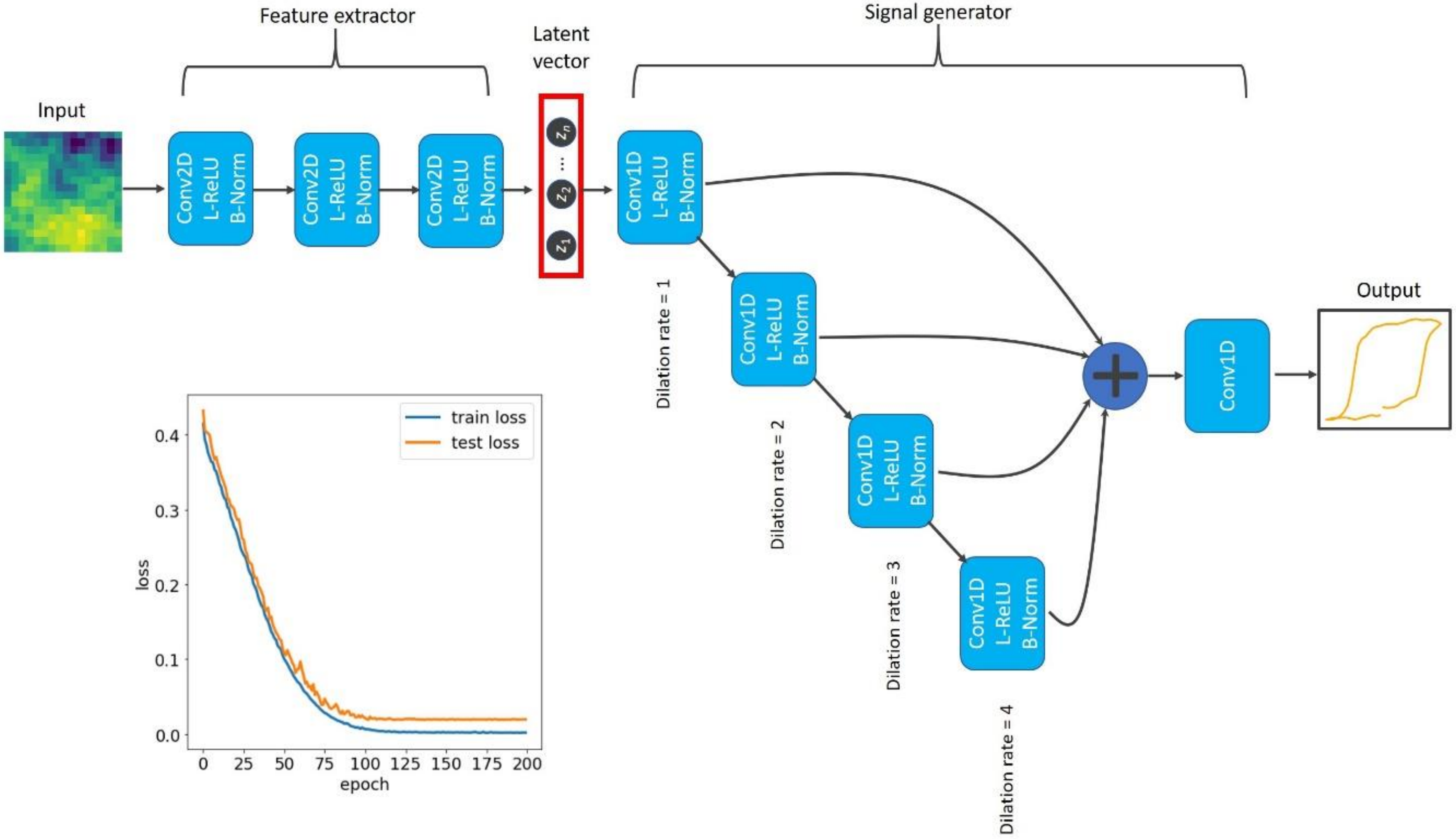


Pinning mechanism





Encoders-Decoders



- Use encoder-decoder architecture to transform local structure to local spectra
- And spectra to images
- Predictive within the image

Latent space

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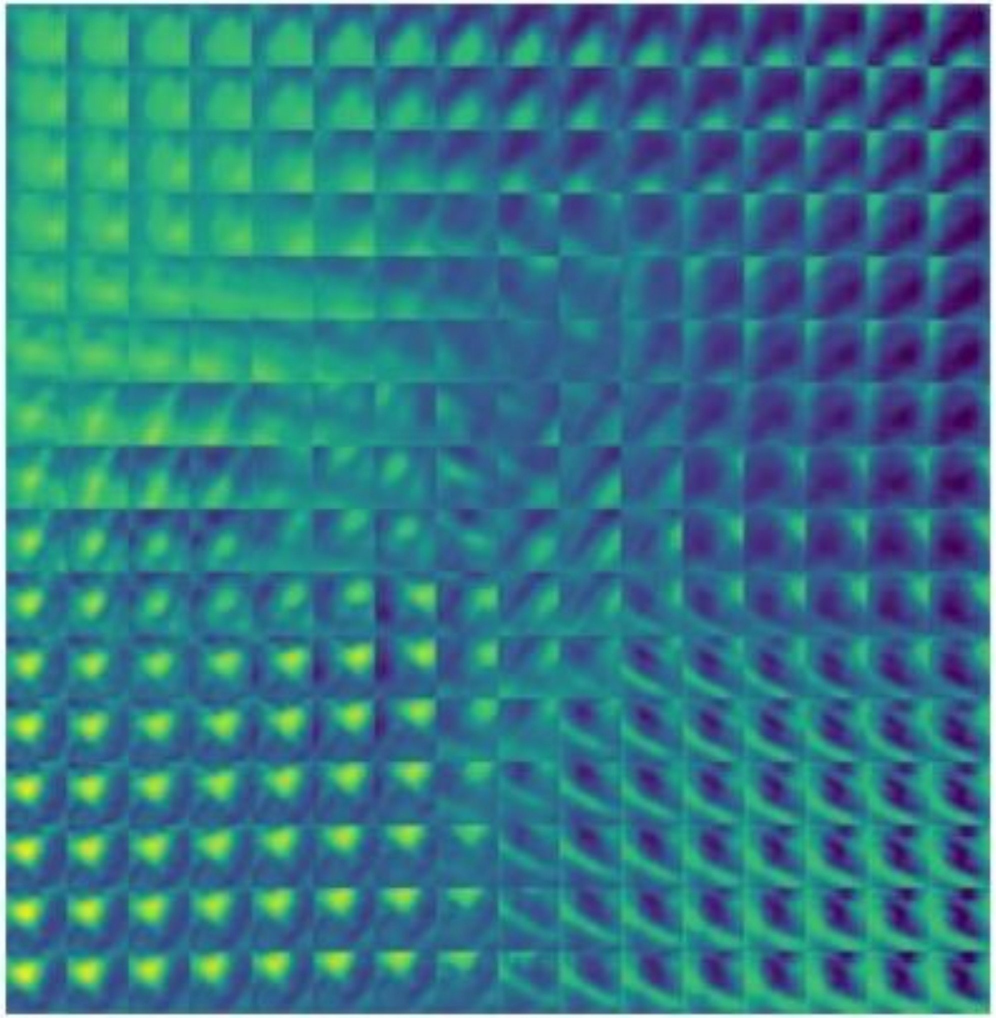
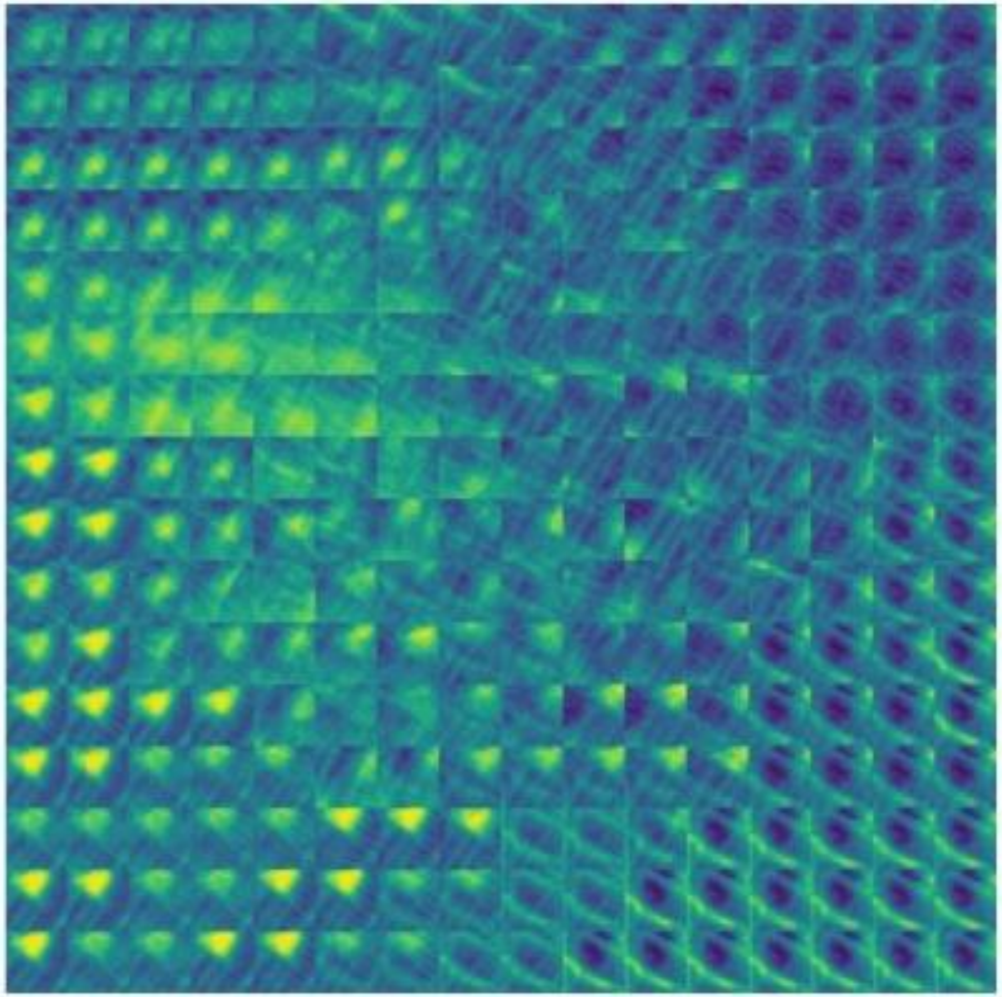




Prediction

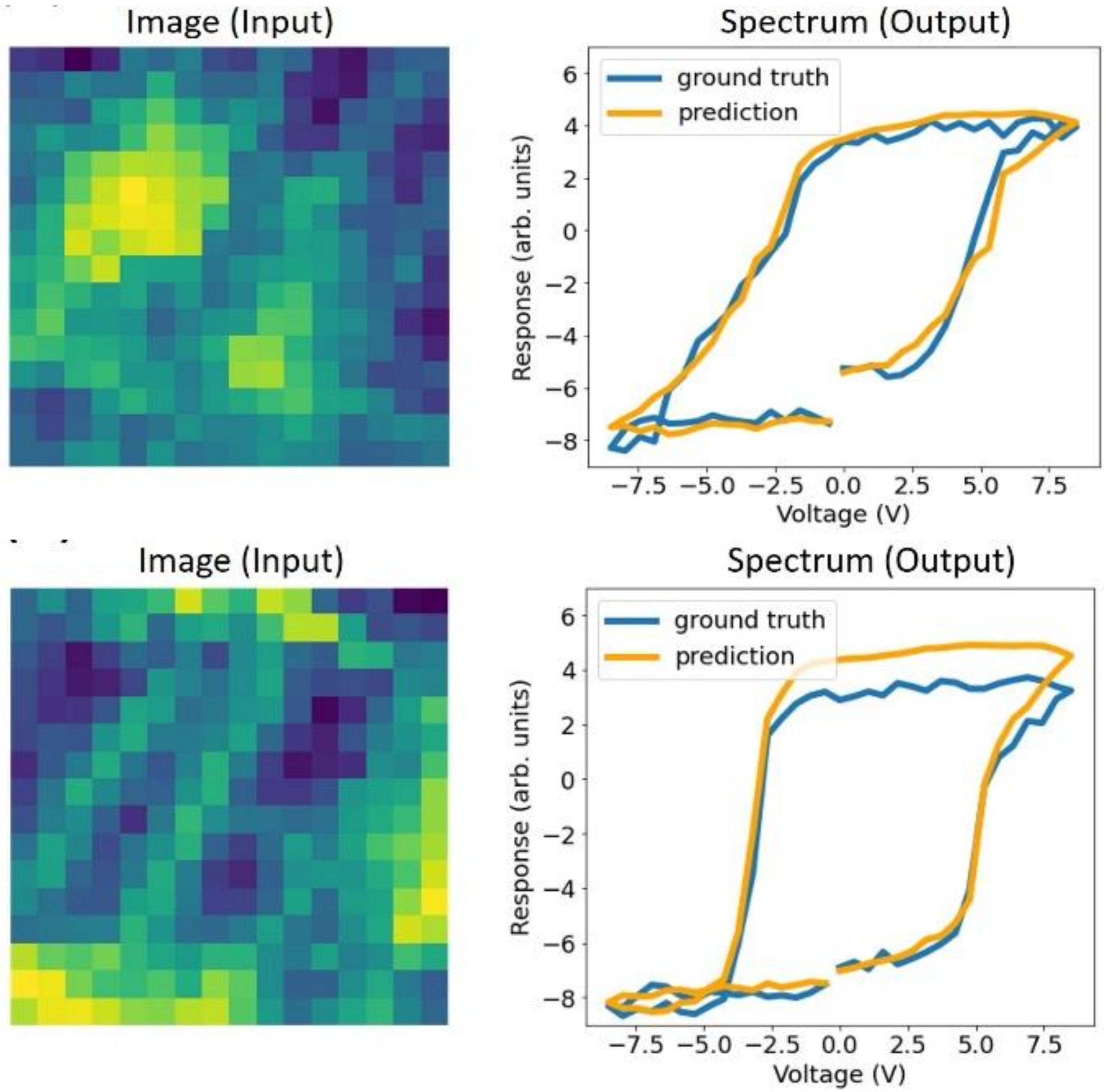
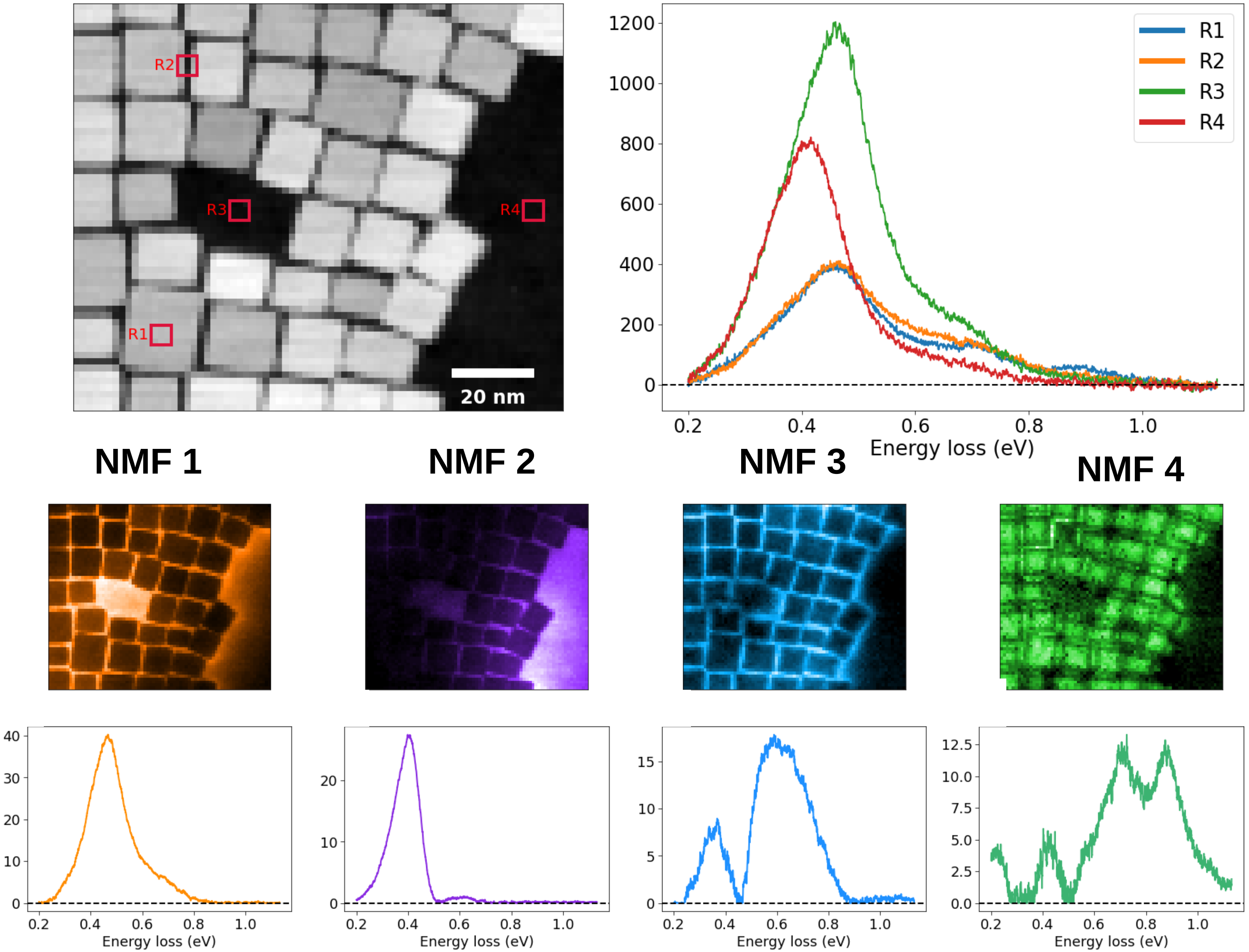
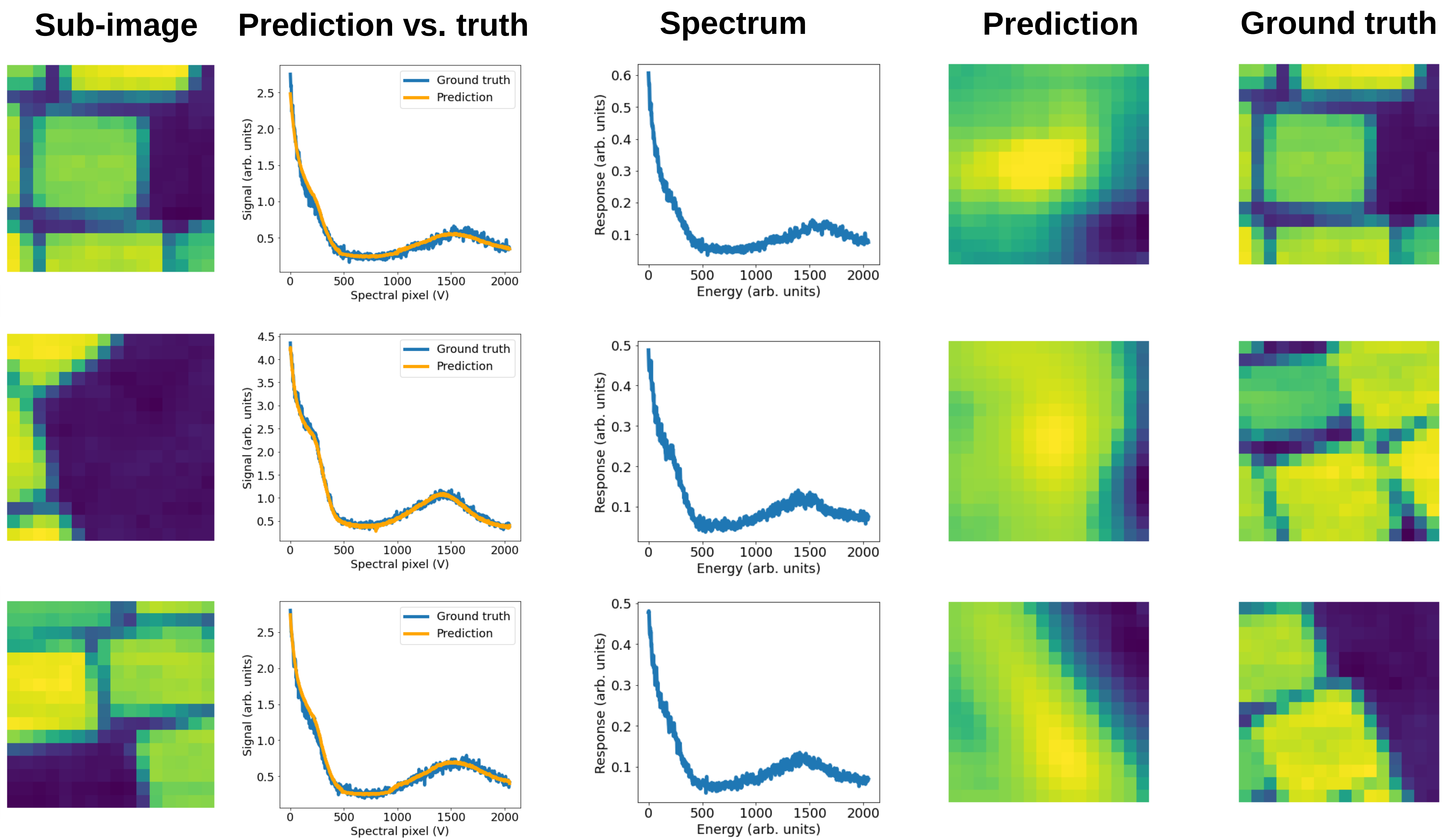


Image (Input)
Spectrum (Output)
ground truth
prediction
Response (arb. units)
Voltage (V)
6
4
2
0
−2
−4
−6
−8
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
Image (Input)
Spectrum (Output)
ground truth
prediction
Response (arb. units)
Voltage (V)

Plasmonic nanoparticles

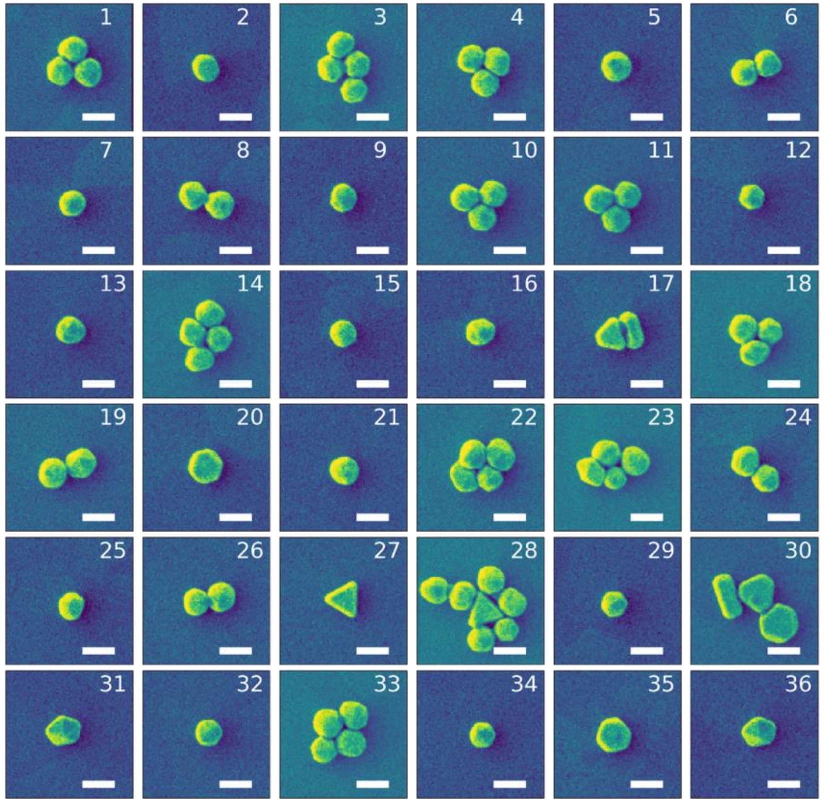


Encoders-Decoders

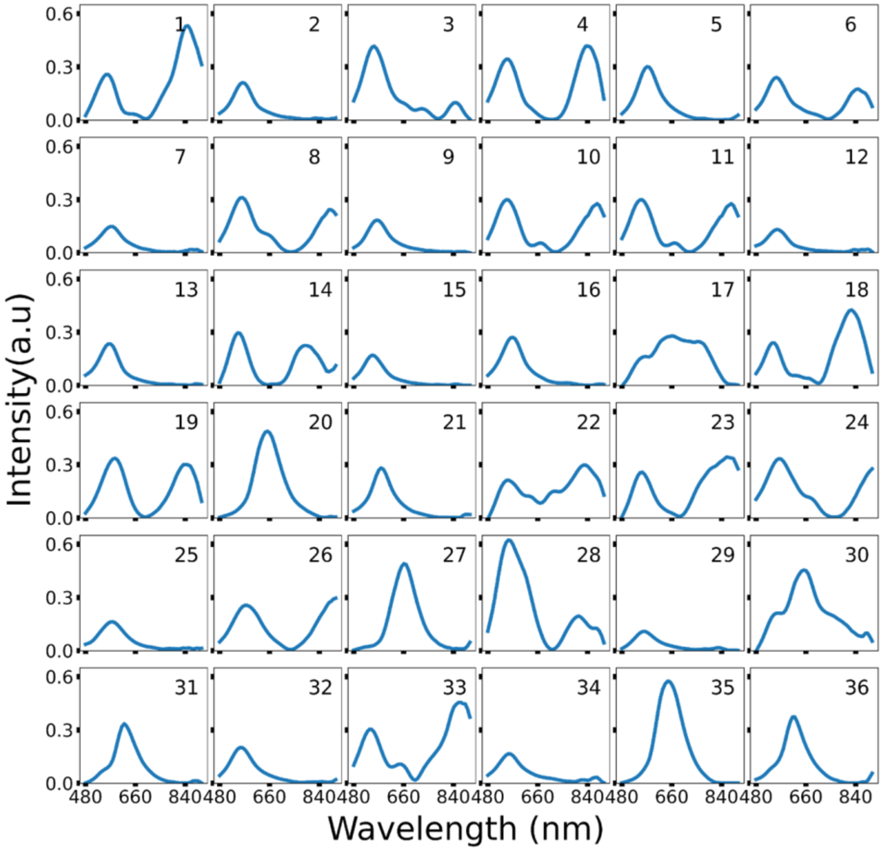


Dual VAE: structure-property relationships

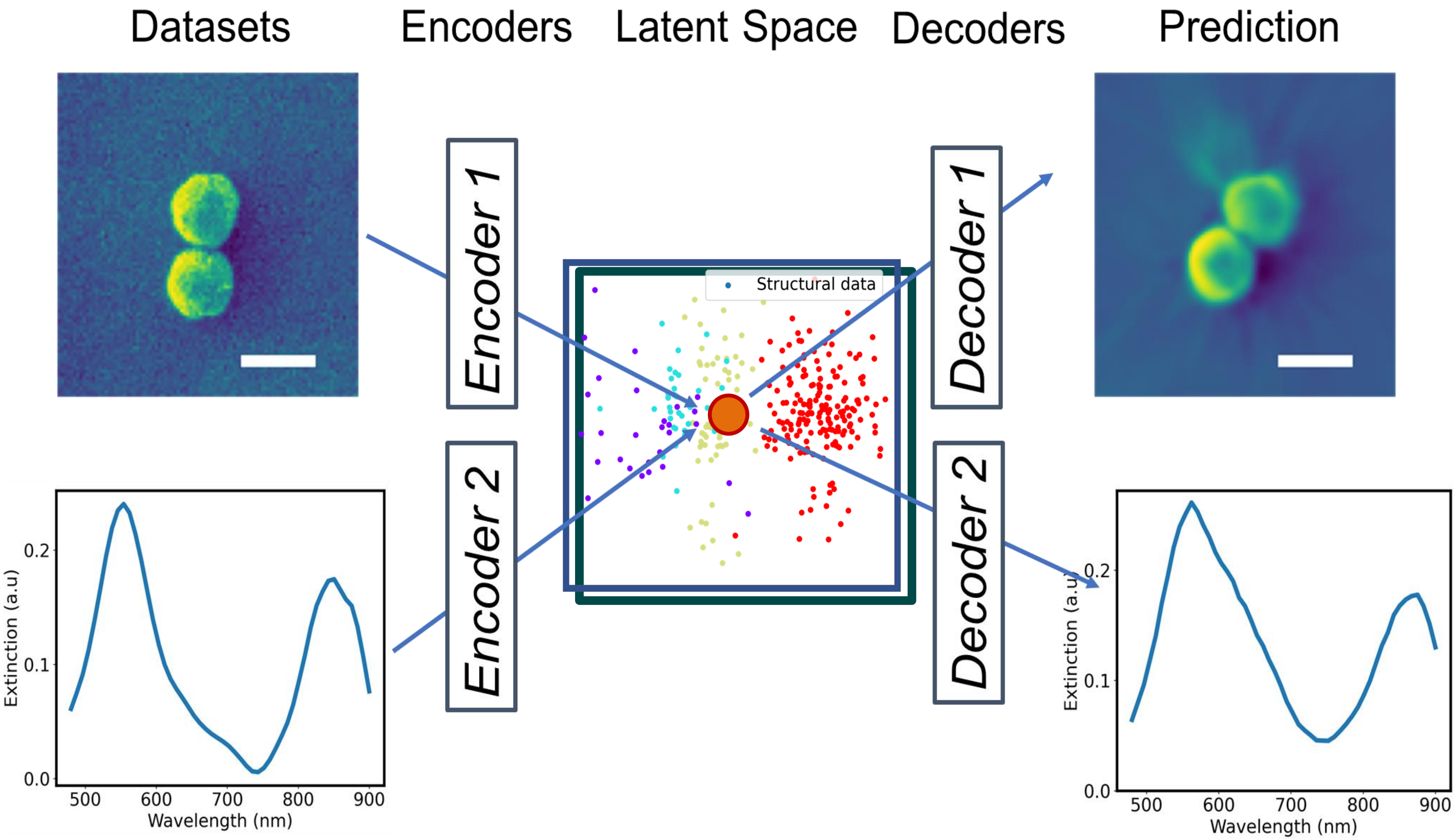
SEM images: "Structure Information"



Hyperspectral microscope: "Property Information"



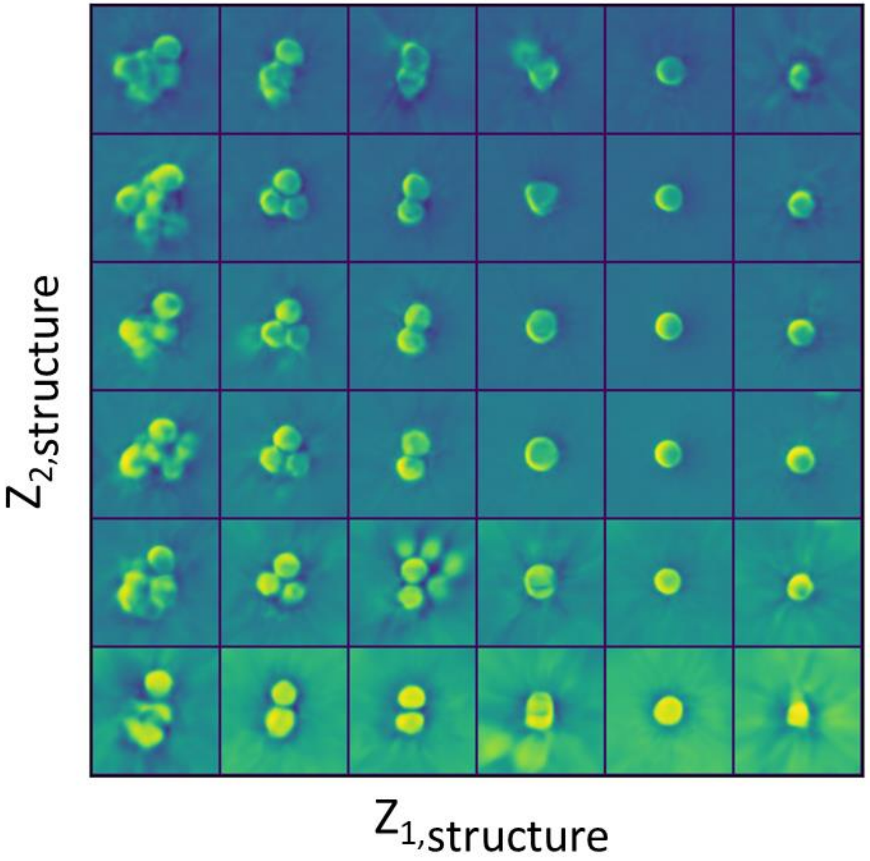
Dual VAE

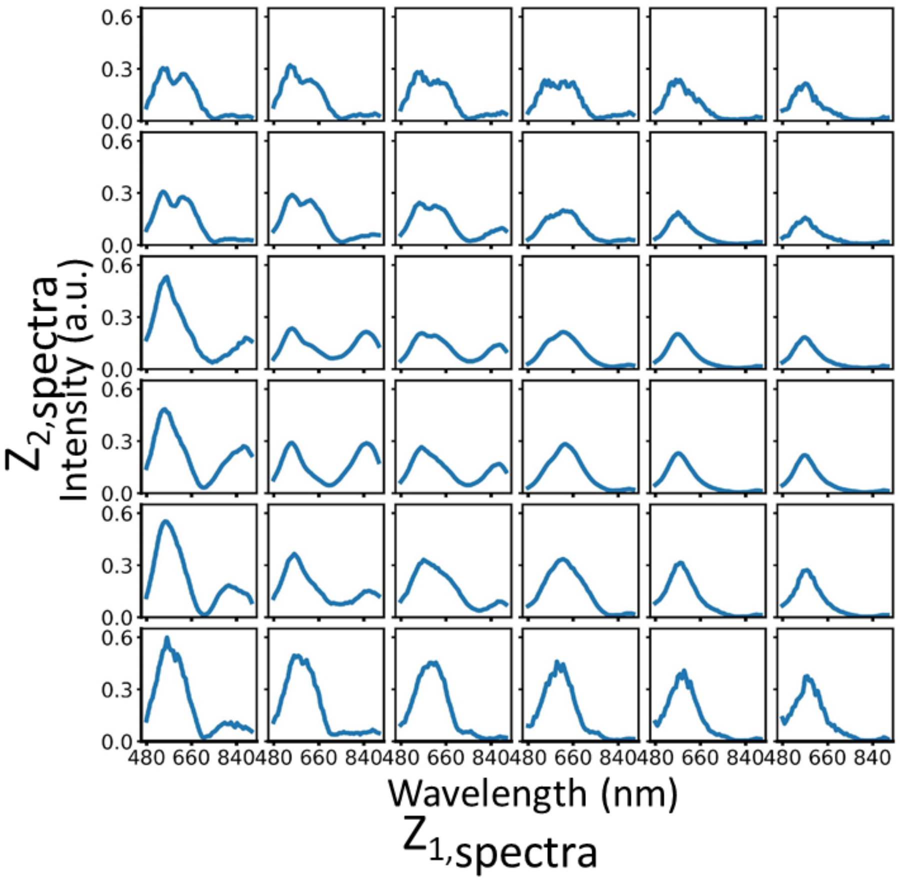

Datasets
Encoders
Latent Space
Decoders
Prediction
Encoder 1
Encoder 2
Structural data
Decoder 1
Decoder 2
Extinction (a.u)
Wavelength (nm)
0.0
0.1
0.2
500
600
700
800
900

Dual VAE: Latent Represnetations

Manifold Representation

Changing in particle shape





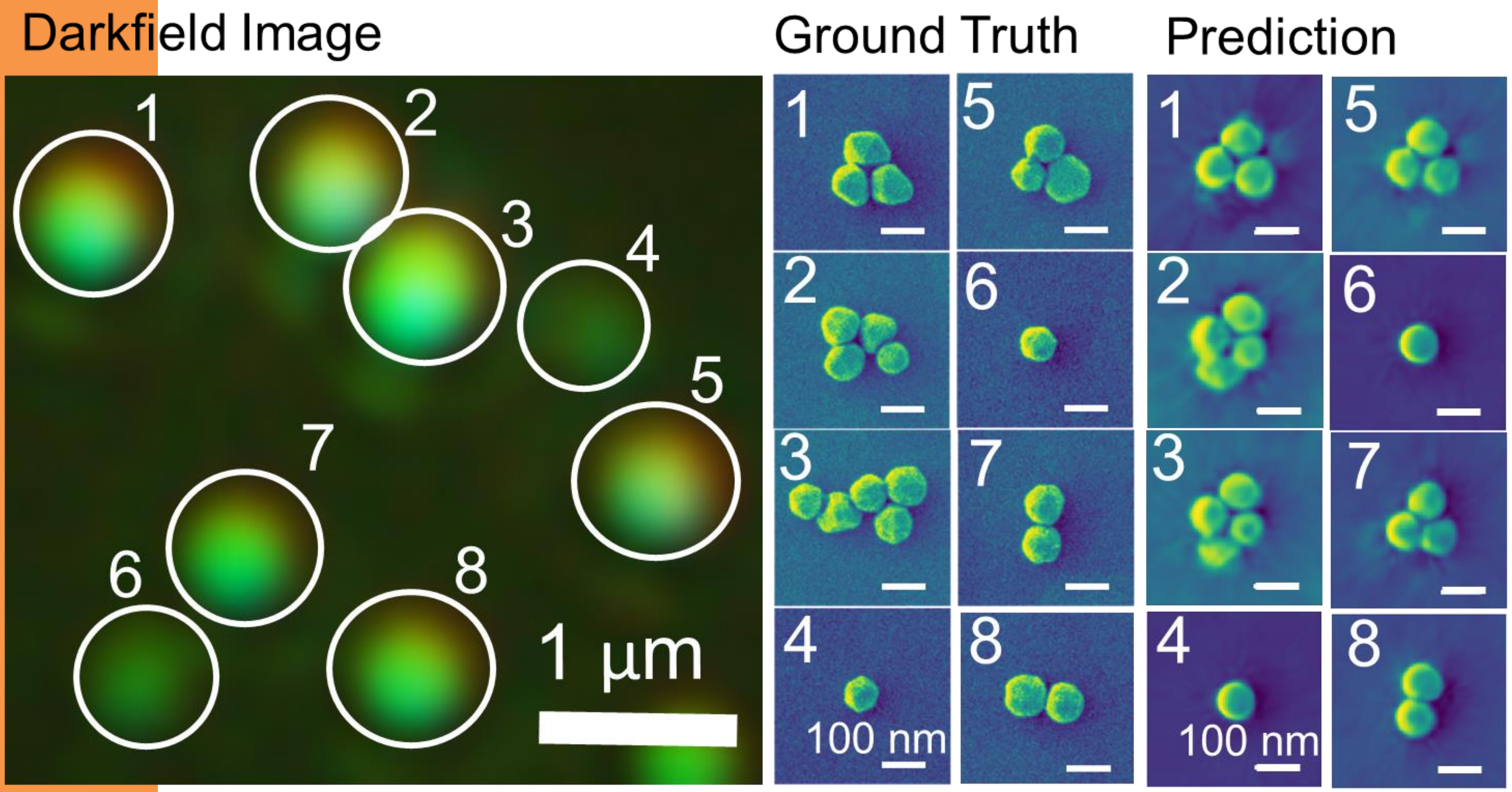
Changing in spectrum shape

increasing in particle number in a cluster

increasing in the peak intensity

Dual VAE: Predictions

Example



Overall Particles