THE UNIVERSITY of TENNESSEE KNOXVILLE

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

(Variational) Autoencoders

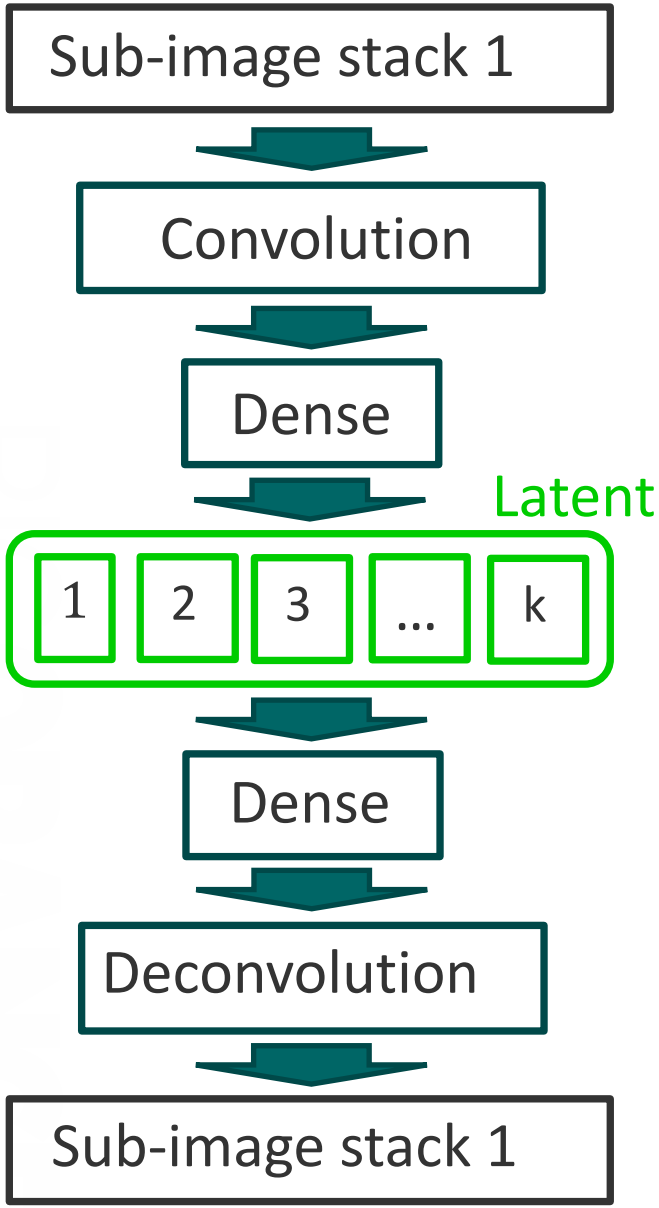
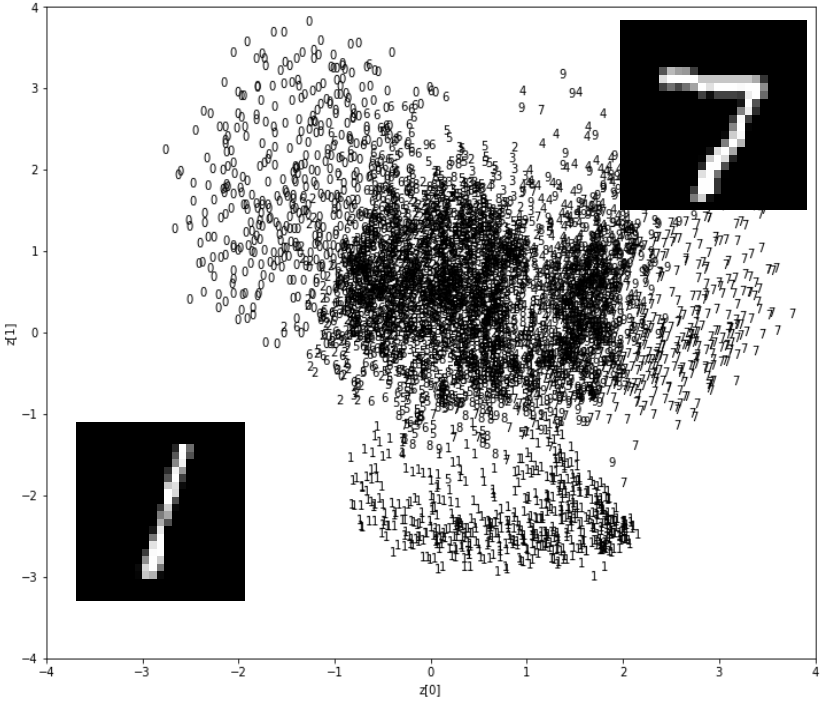
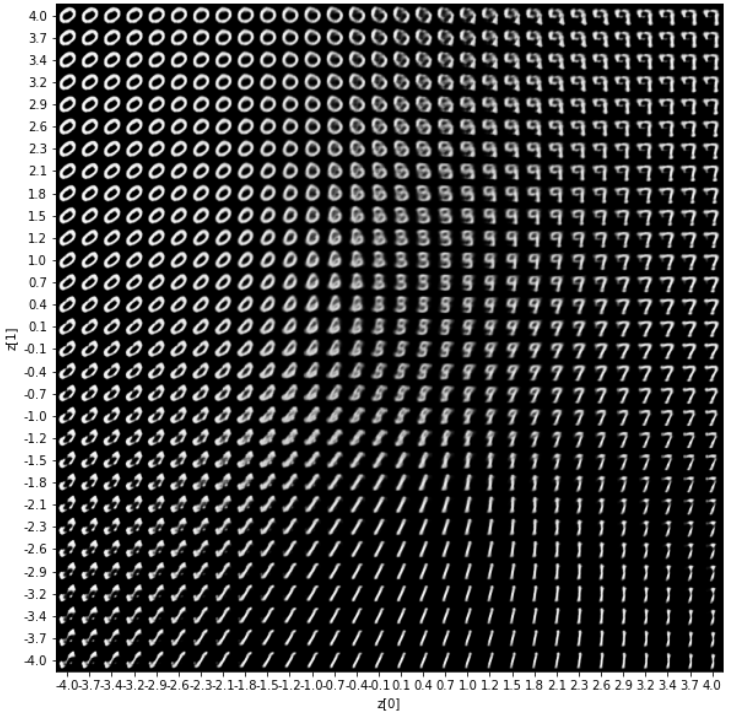


Image → Latent space

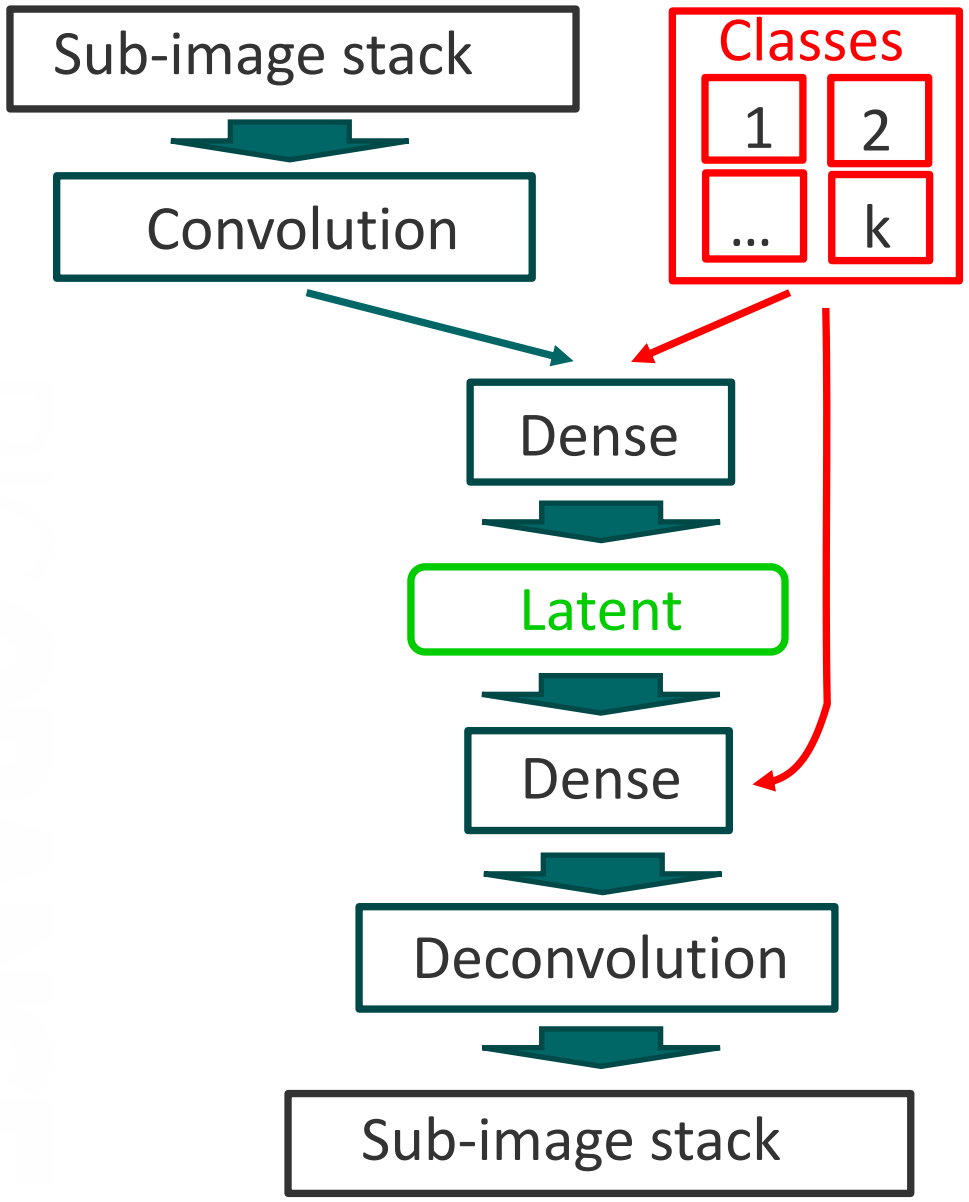


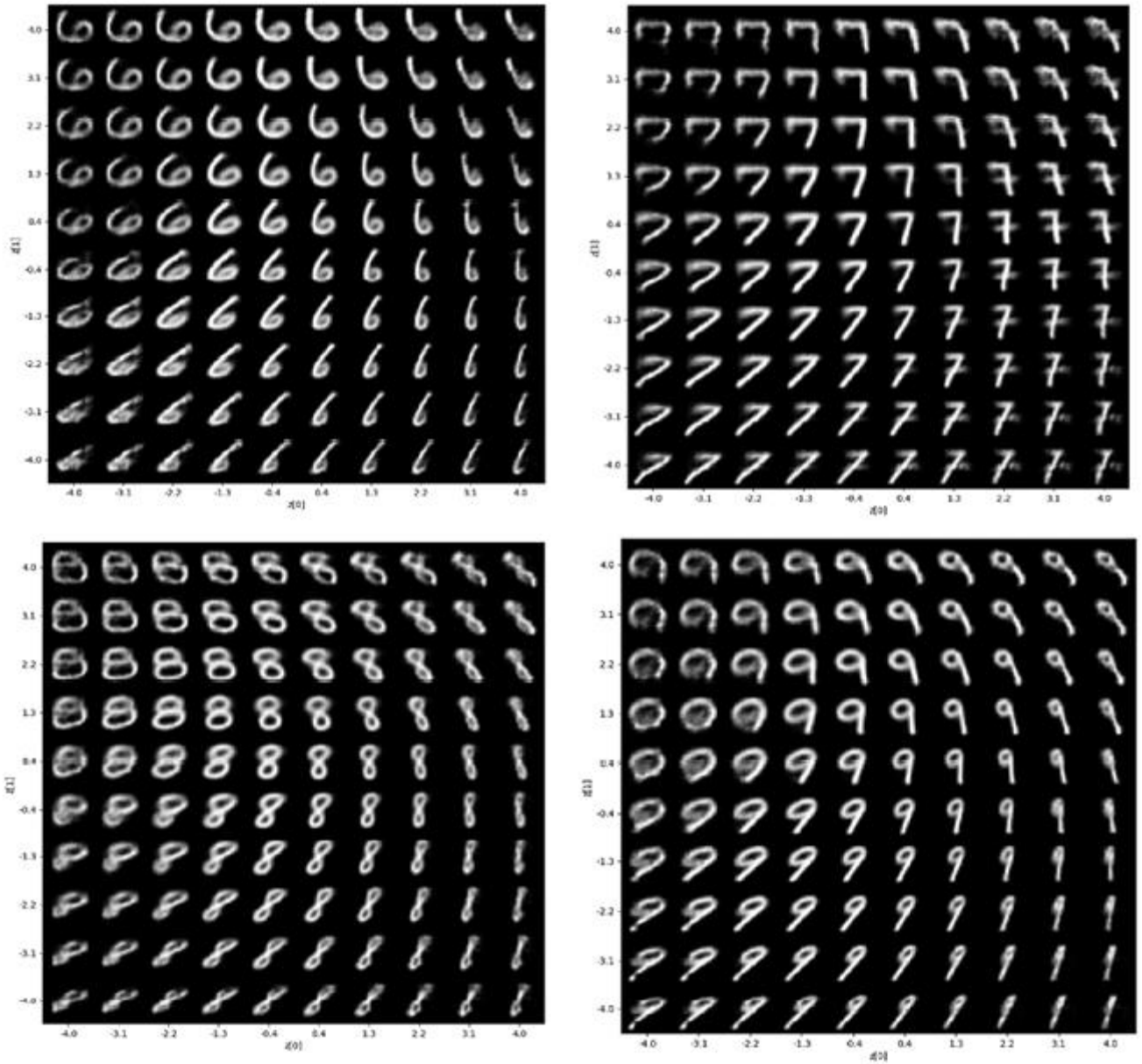
Latent space → Image



- Encoding: Latent distribution
- Decoding: Latent representation
- Disentanglement of representations
- Invariances: rotation, translation, scale
- Conditional, joint, and semi-supervised VAEs

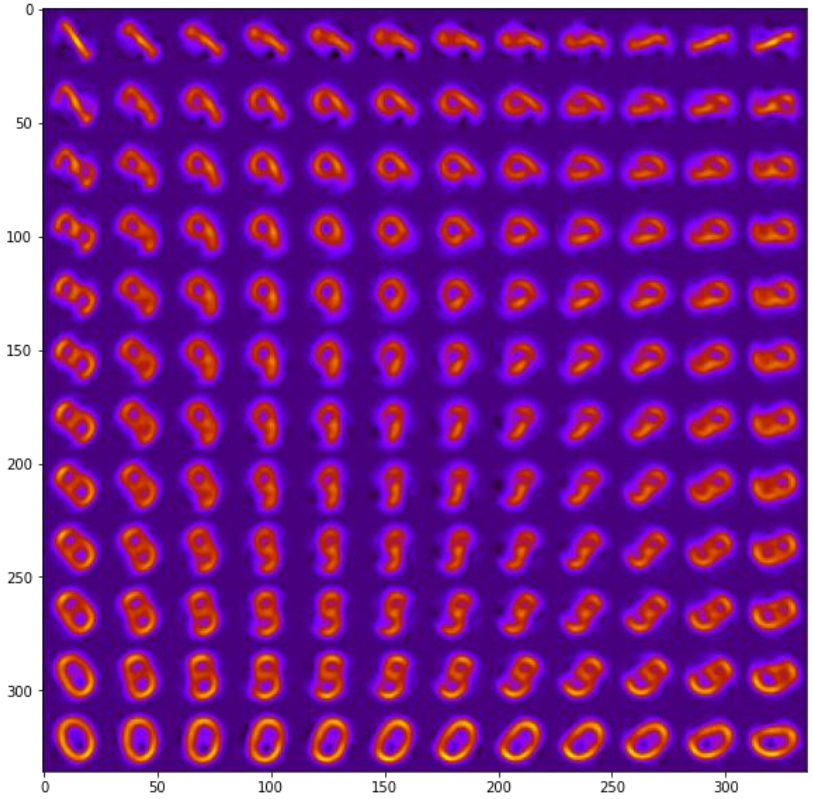
Disentanglement of representations



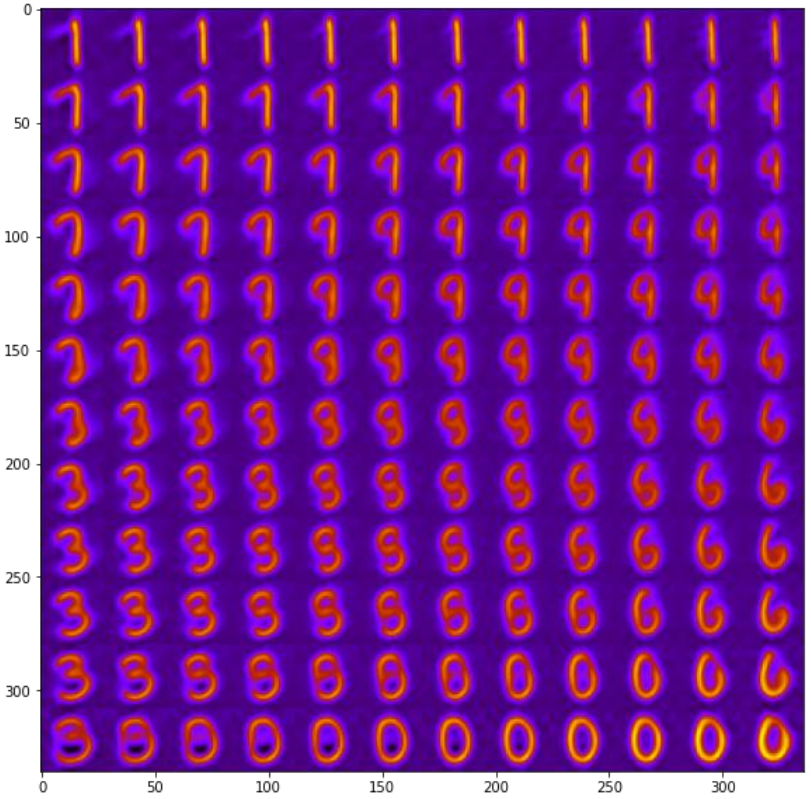


Invariances in VAEs

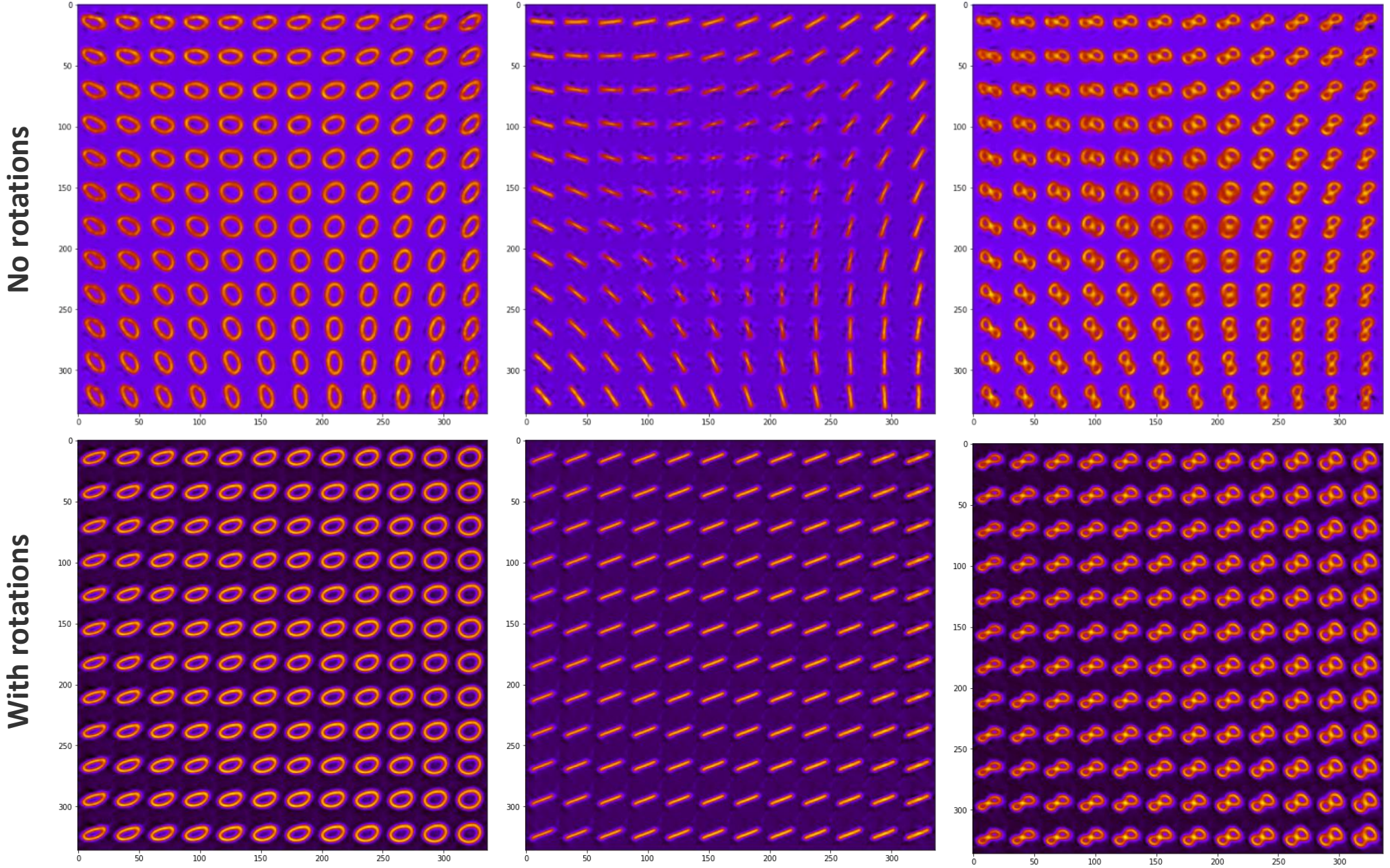
VAE



rVAE



Invariances in VAEs



What can (unsupervised) classification give us

- Our research deals with complex data sets containing information on physics of objects we seek to understand
- This can be spectral data sets (EELS in STEM, CITS in STM, complex spectroscopies in PFM) or single, multimodal, or hyperspectral images
- Often, we seek approaches to reduce dimensionality and explore similarities in these data sets.

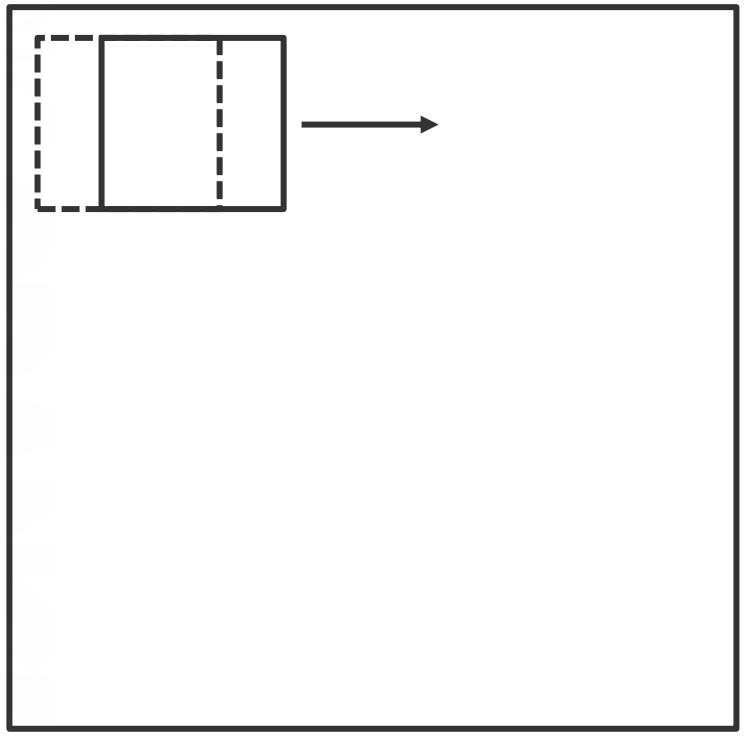
- When working with such data sets, two things matter: descriptors and ML method
- In analysis of EELS or CITS data, very often our descriptor is just the spectrum at each pixel. Typical analysis will be either linear or non-linear dimensionality reduction or clustering:
  - Linear dimensionality reduction: PCA, NMF, BLU
  - Clustering: k-means, GMM
  - Manifold learning: ISO, UMAP, tSNE, DBSCAN
  - Neural nets: SOFM, AEs, VAEs
- Typical result will be the components (representing behavior), and loading maps representing spatial variability of these behaviors. By construct, components will not depend on the relative spatial positions of pixel.

- What about images?

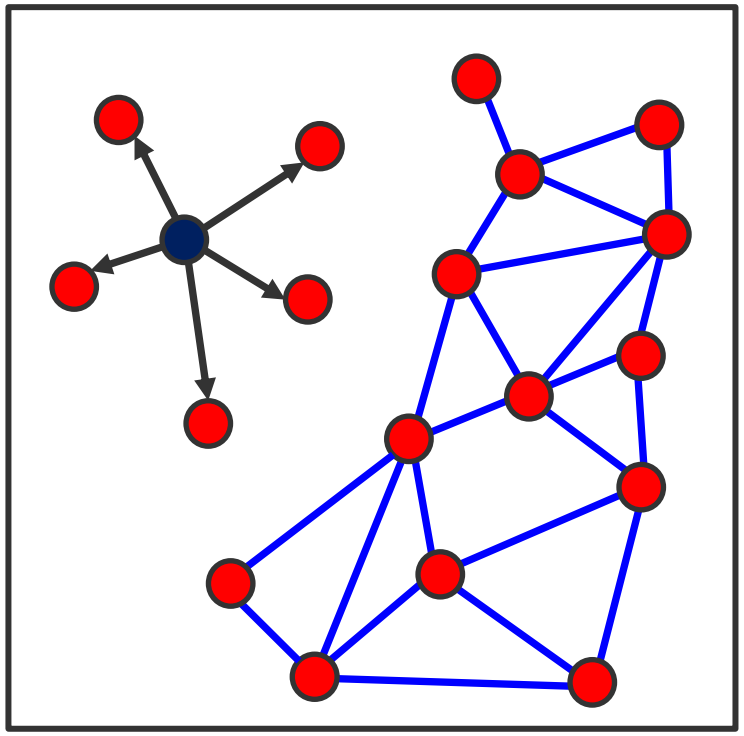
Describing the building blocks

- 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

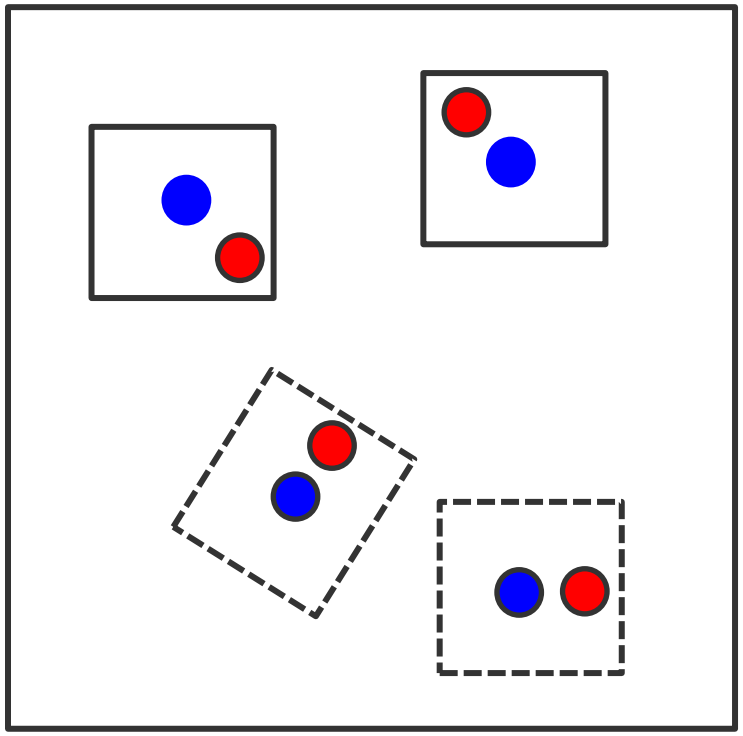
Continuous translational symmetry



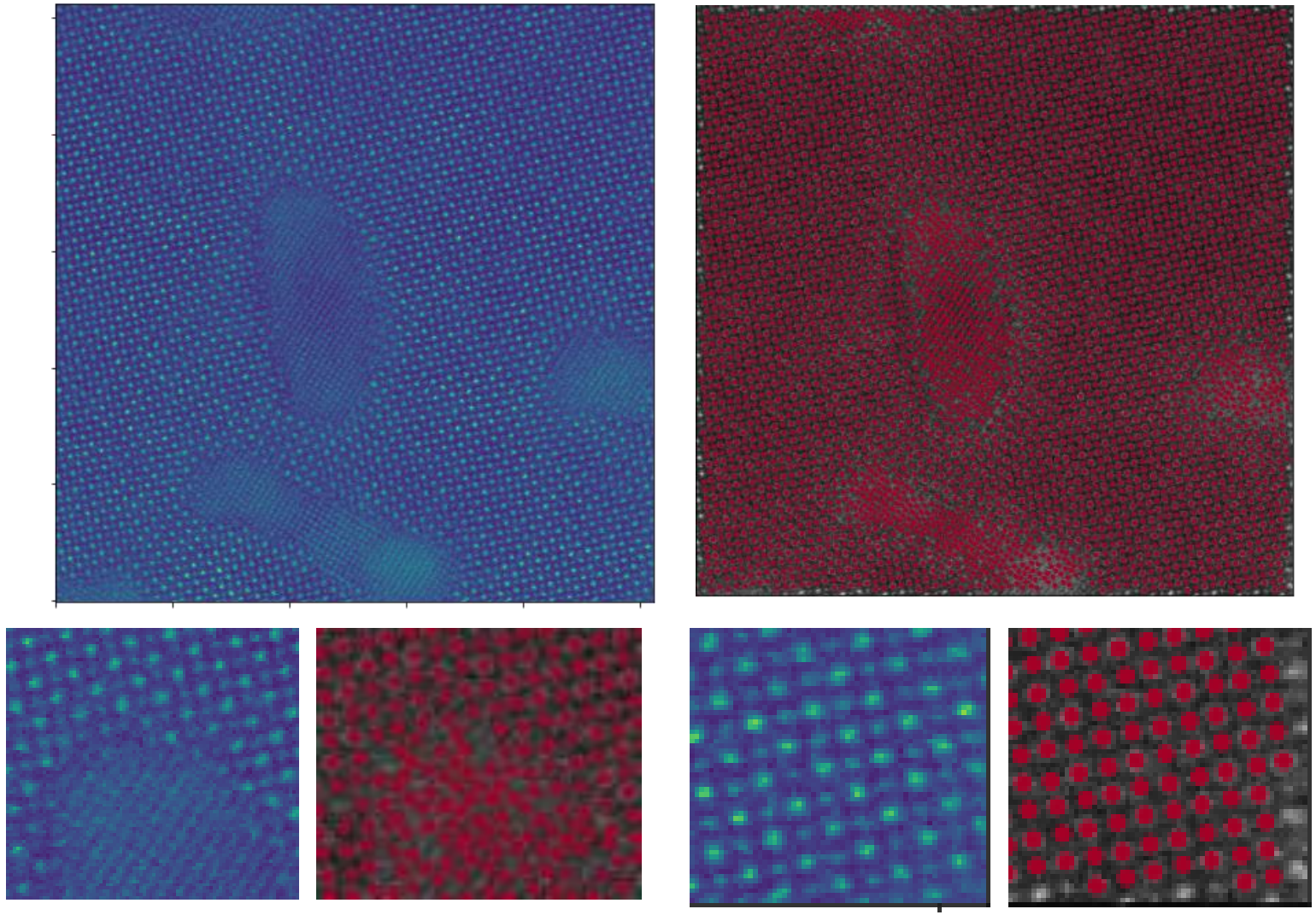
Atom based descriptions



Localized sub-images



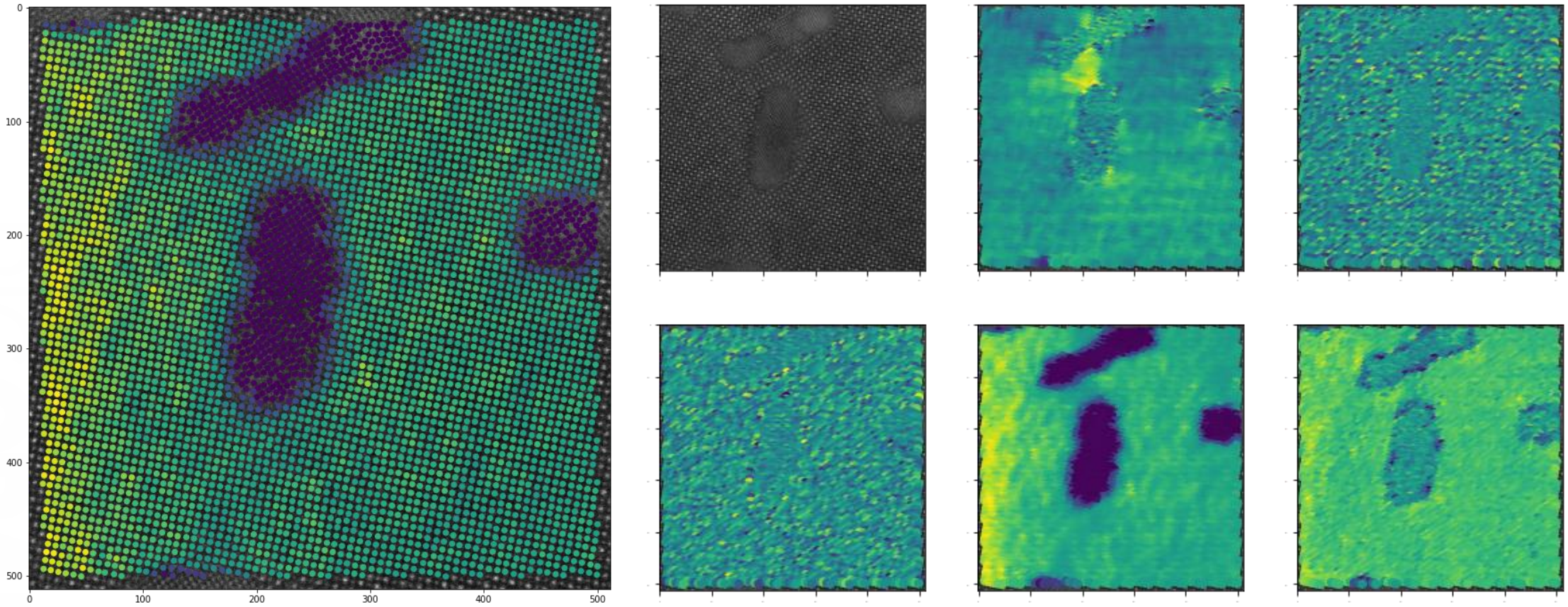
Let's put it all together!



Step 1: Find all atoms (or all that you can) – use maximum finders, blob-log, or DCNNs

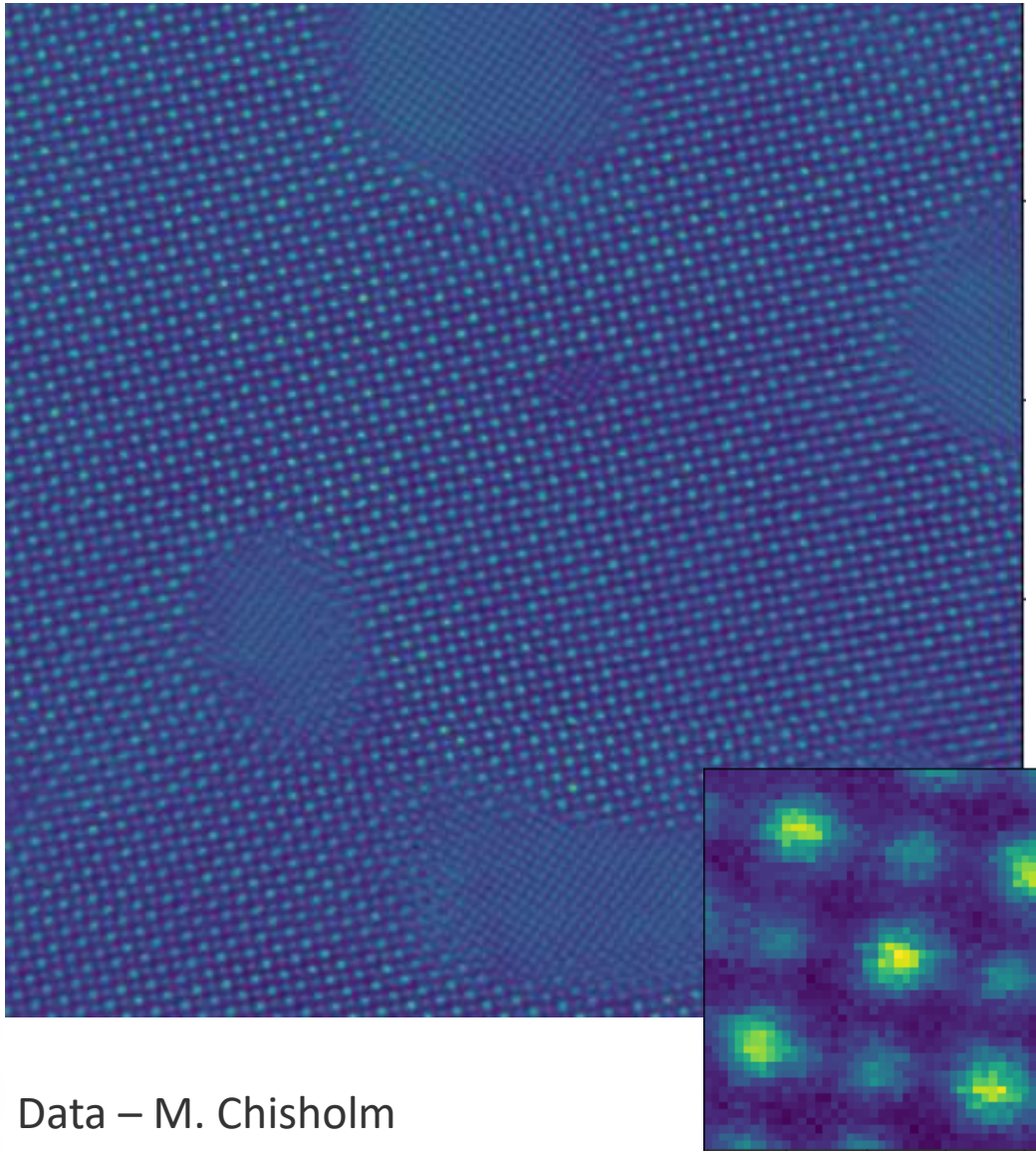
Step 2: Create descriptors – patches centered on atoms. Keep track on what part of image (or stack) it came from

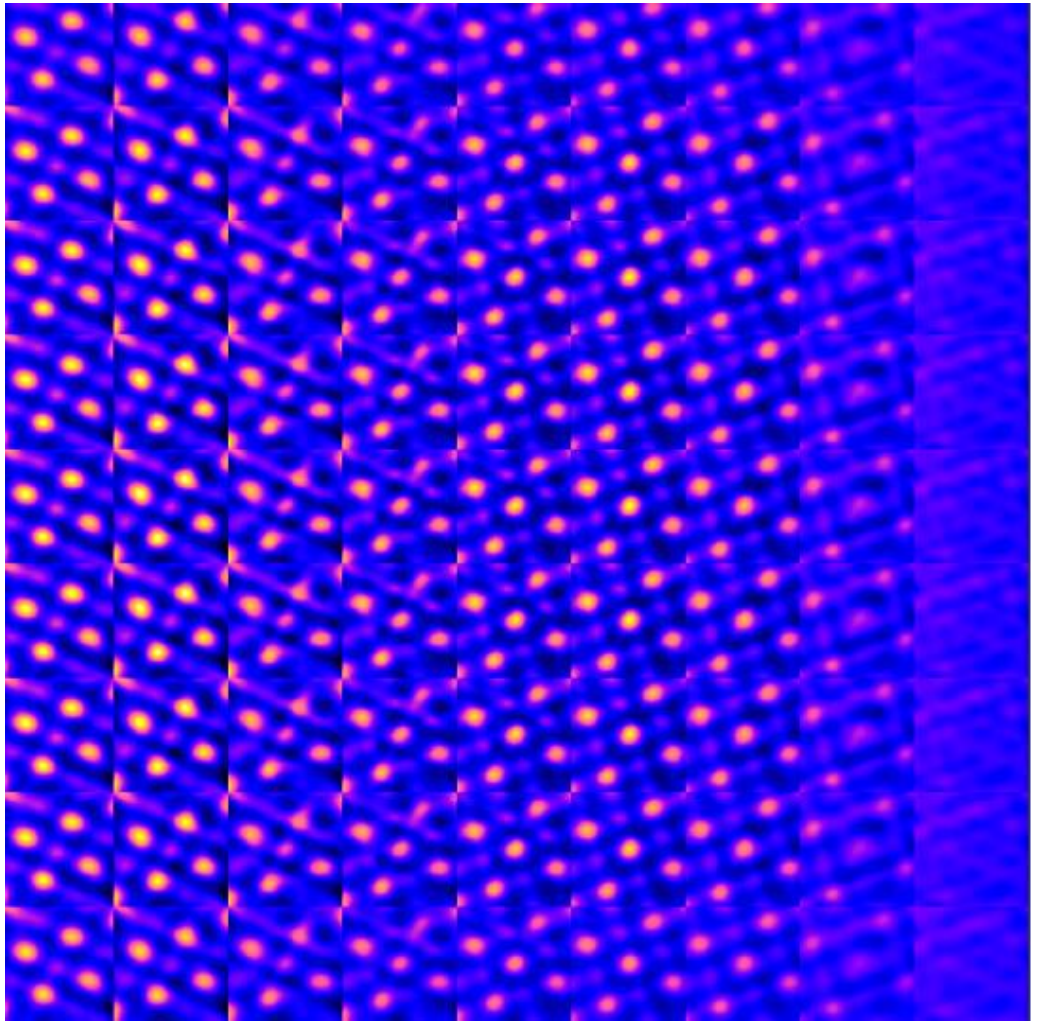
Step 3: rVAE



Output: Latent variable corresponding to local structure of each atomic site. Can be visualized on top of the original atomically resolved image, or as 2D maps (but – not rectangular array!)

Analysis of the NiO-LSMO

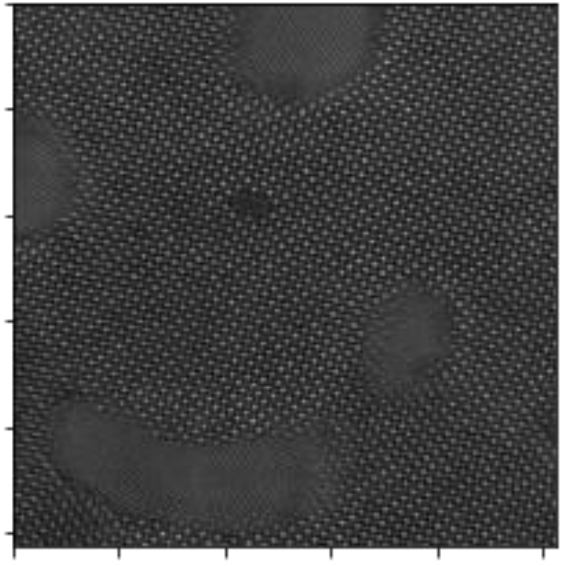




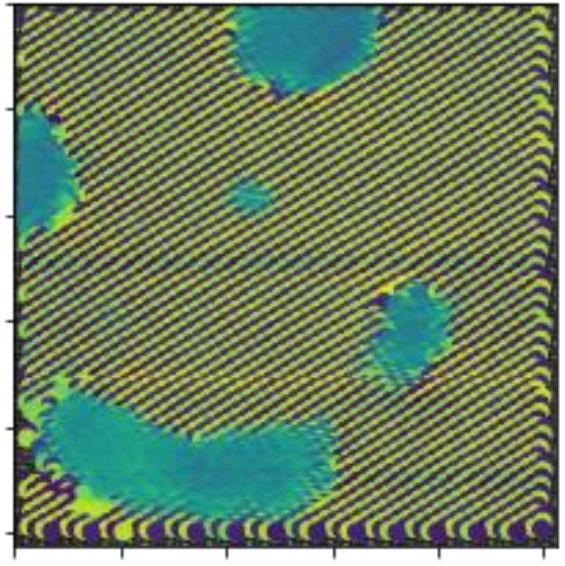
Data – M. Chisholm

Let's look at latent space

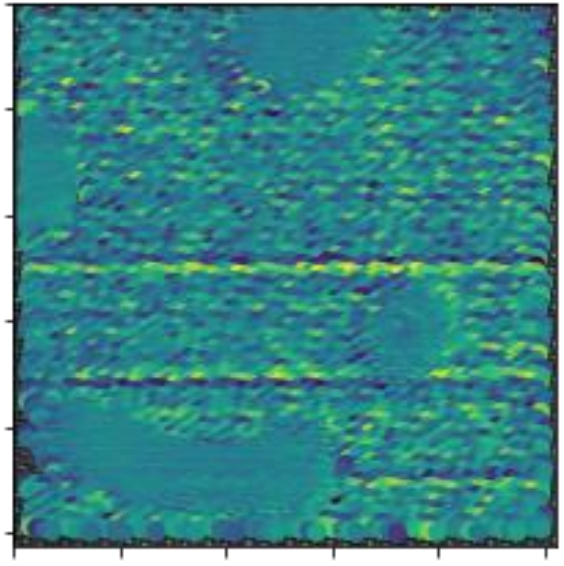
Image



Angle



X Offset



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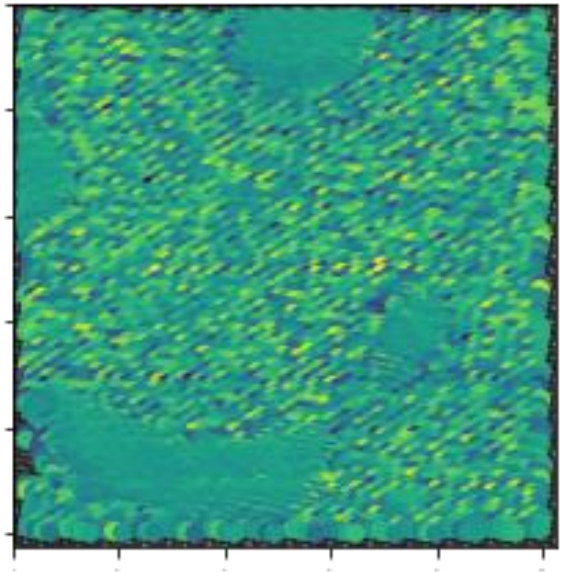
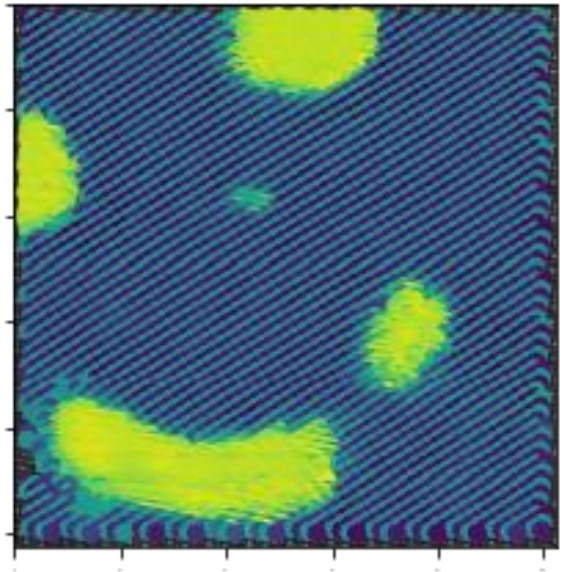
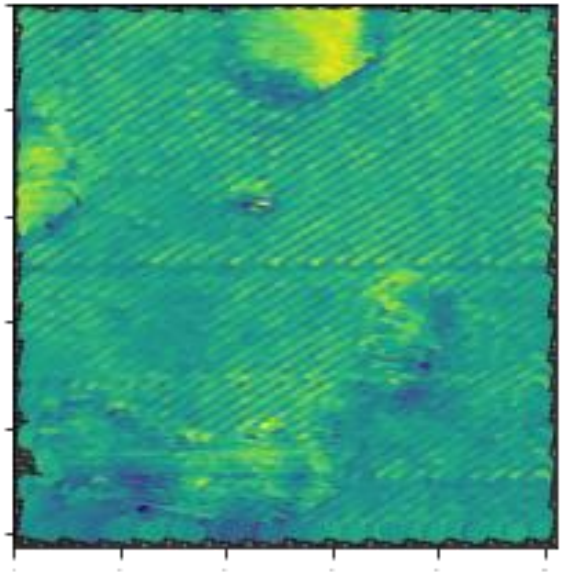


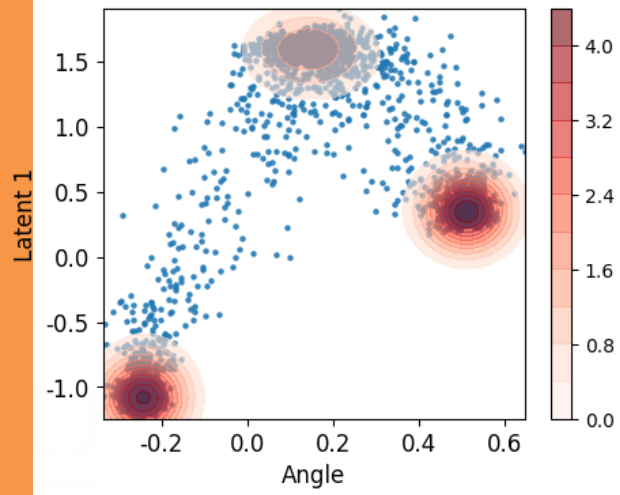
Latent 1

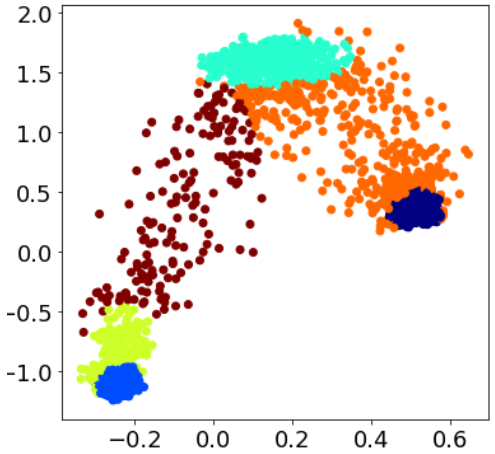


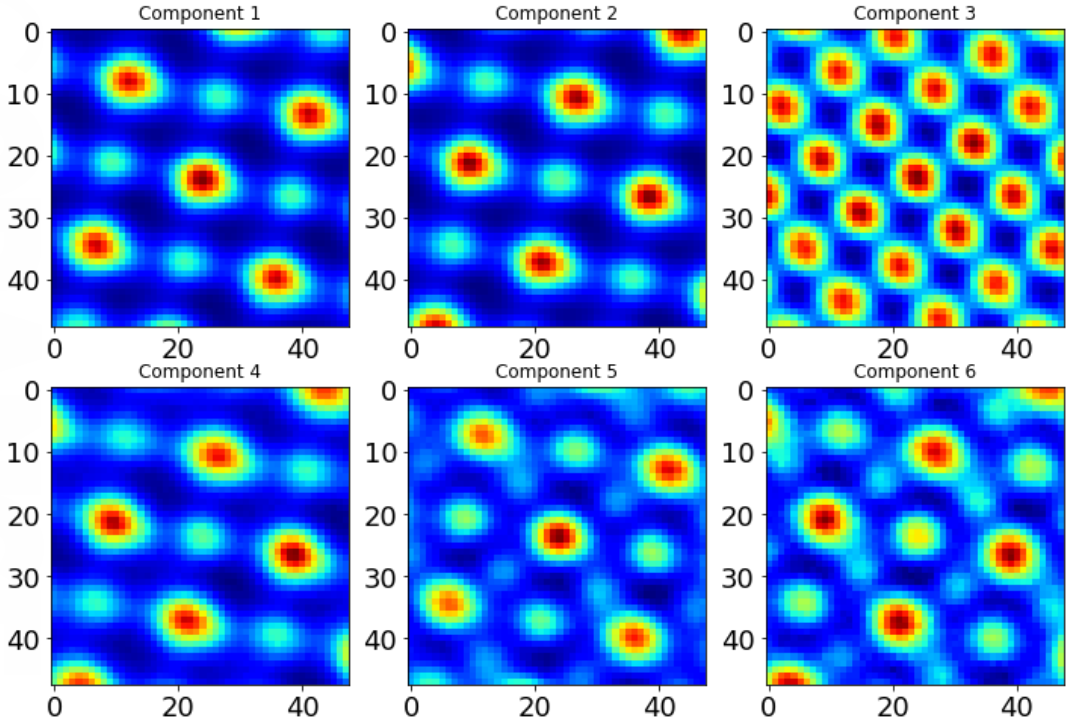
Latent 2



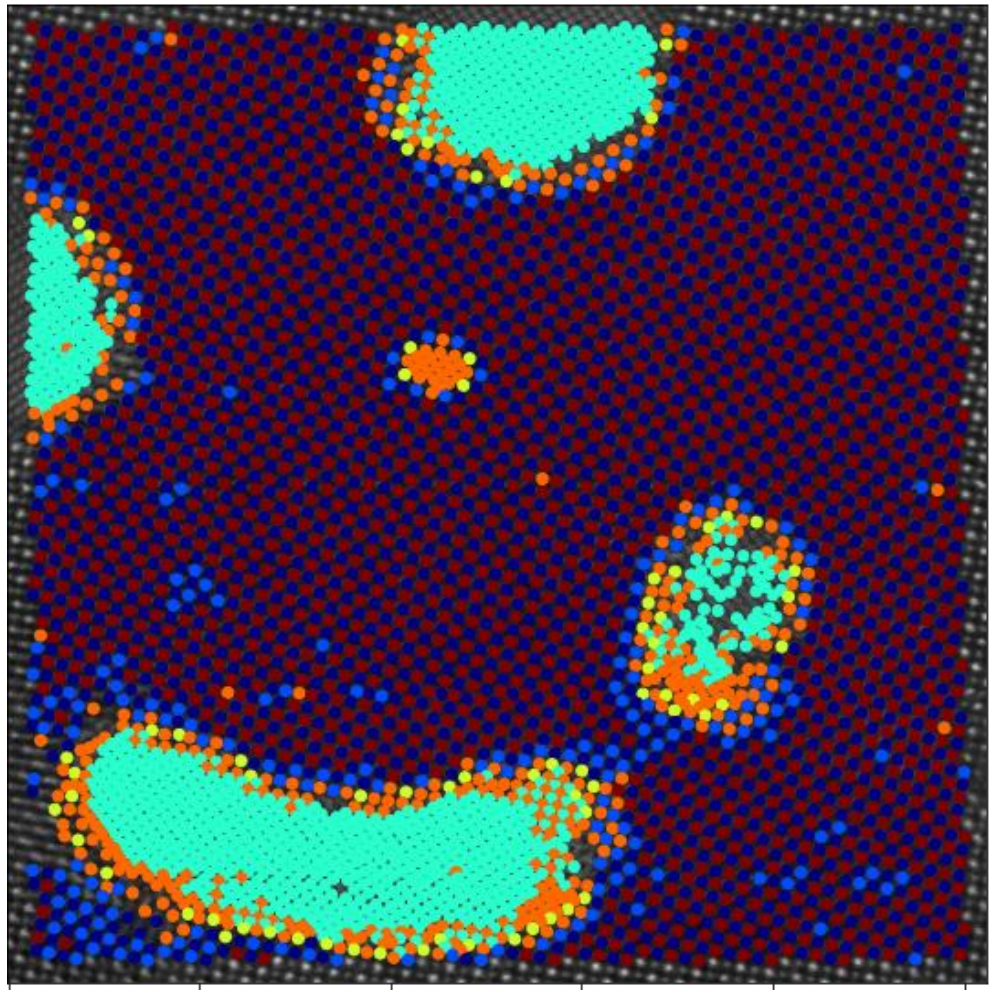
Exploring latent distributions







Labeled image

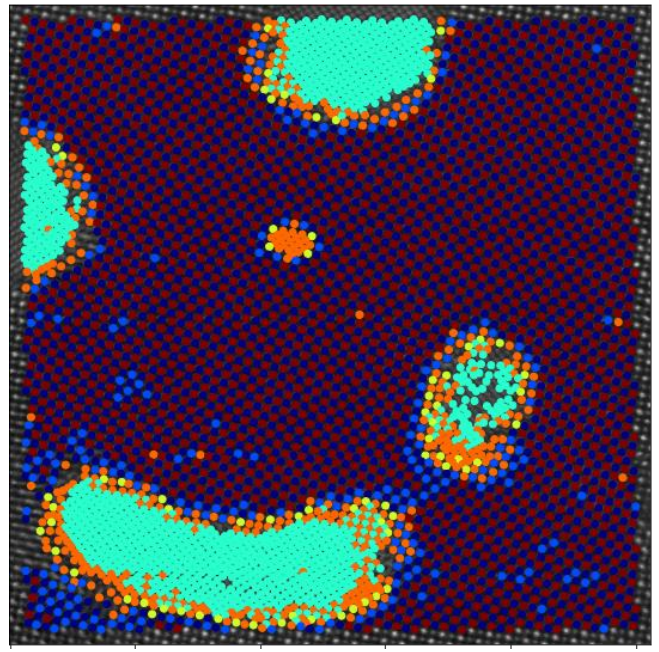


- Classes and variability are mixed in a single latent space
- Disentangling of representation

That's where the jVAE has come from

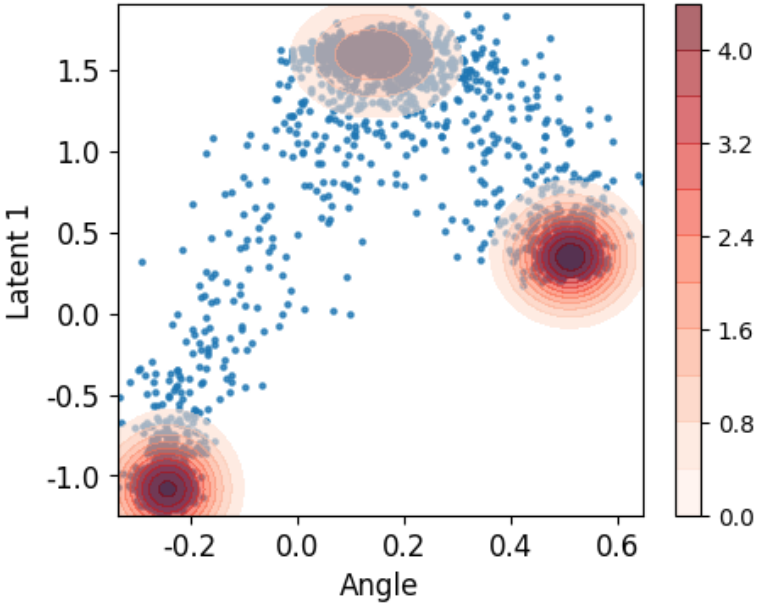
Currently, we have variants of invariant VAE that include:

- Convolutional or dense layers (reconfigurable via **kwargs)
- Rotational invariance
- With and without offsets (as latent variables)
- Multilayer inputs

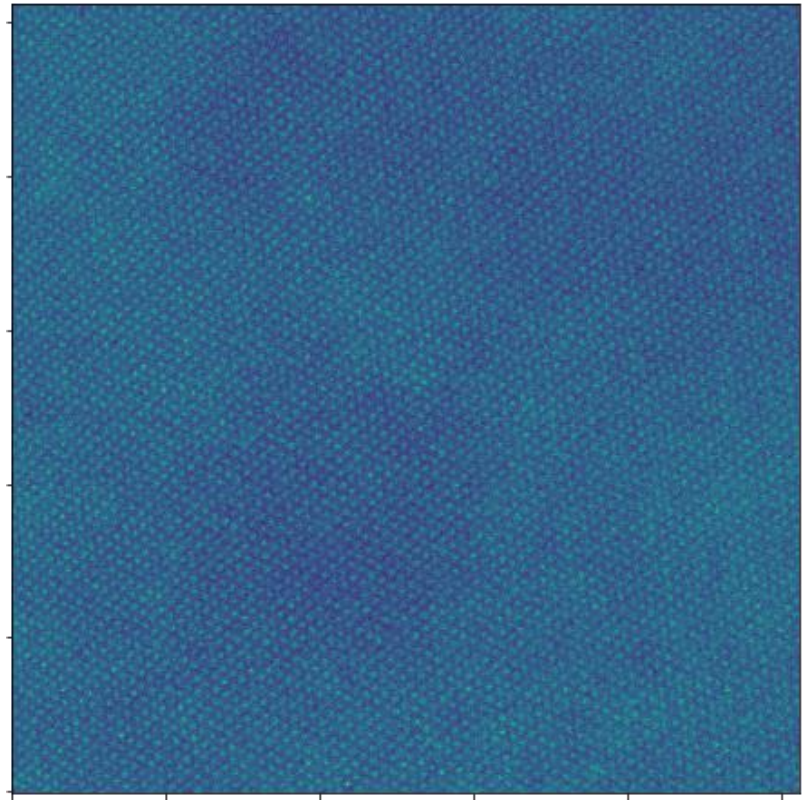


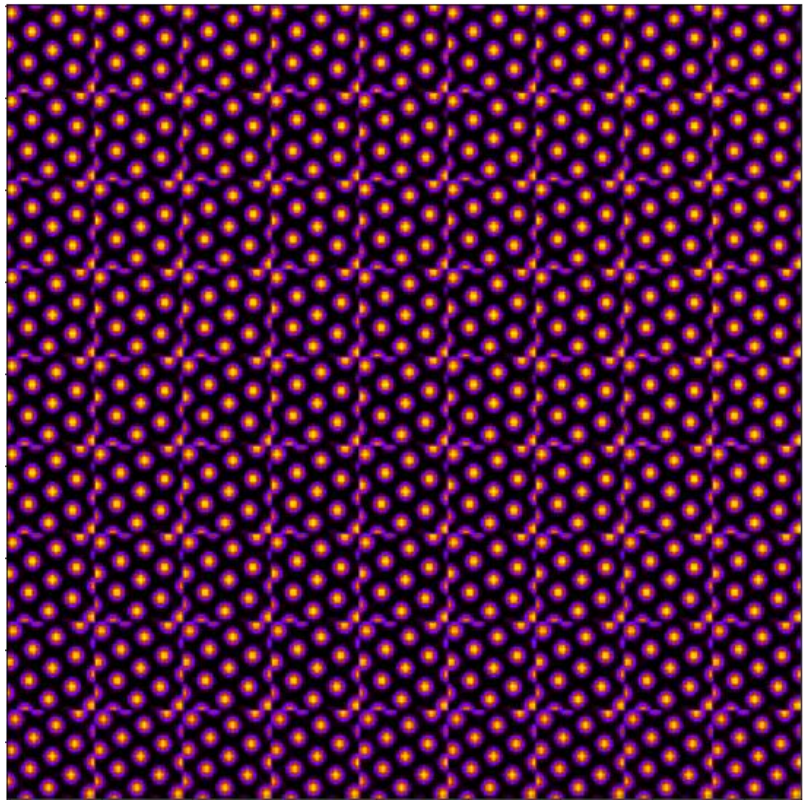
However, our rVAE collects everything in a single latent space. Realistically, very often we deal with system where we expect the presence of finite number of classes that may be known, partially known, or unknown, with certain continuous traits within classes.

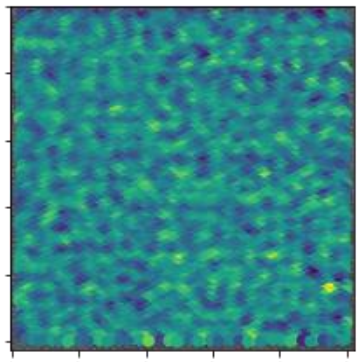
- **Graphene and MX2:** structural units (discrete) and strain states
- **Crystalline solids:** phases and ferroic variants, strain states
- **Plasmonic EELS:** particle spectra, off-particle spectra, edge states
- **CITS:** lattice and defects, strain states

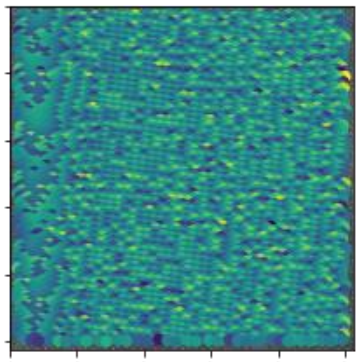


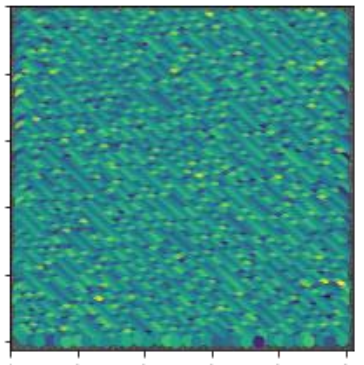
Out of curiosity: single crystal?

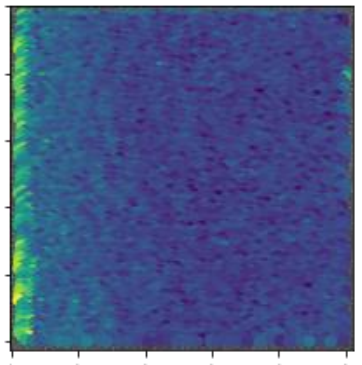


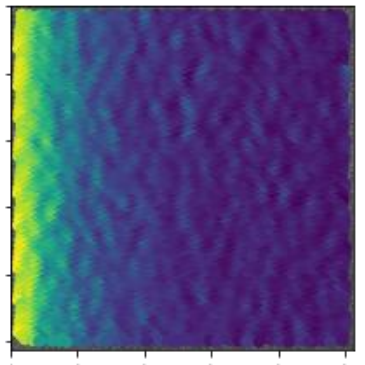






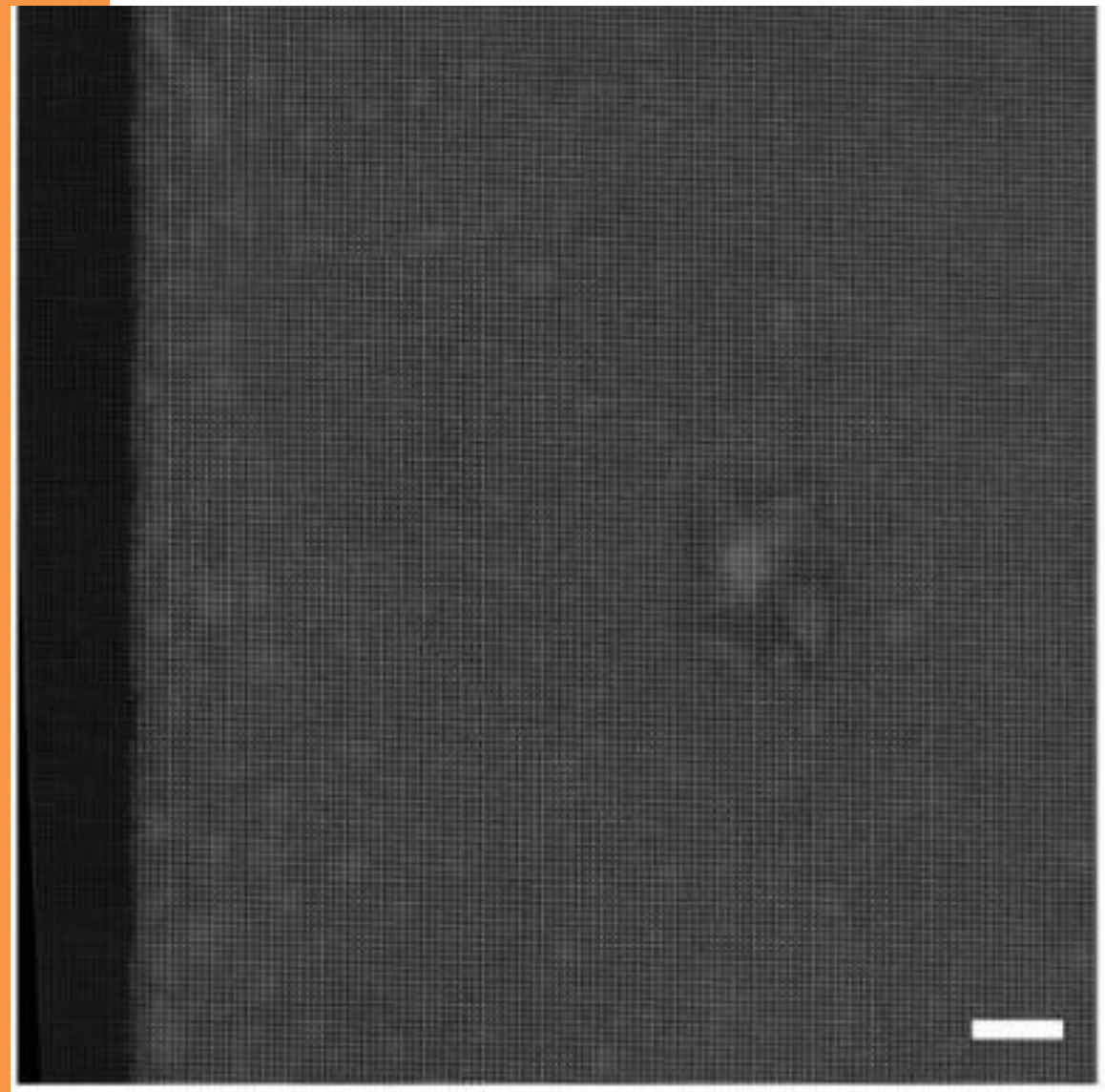




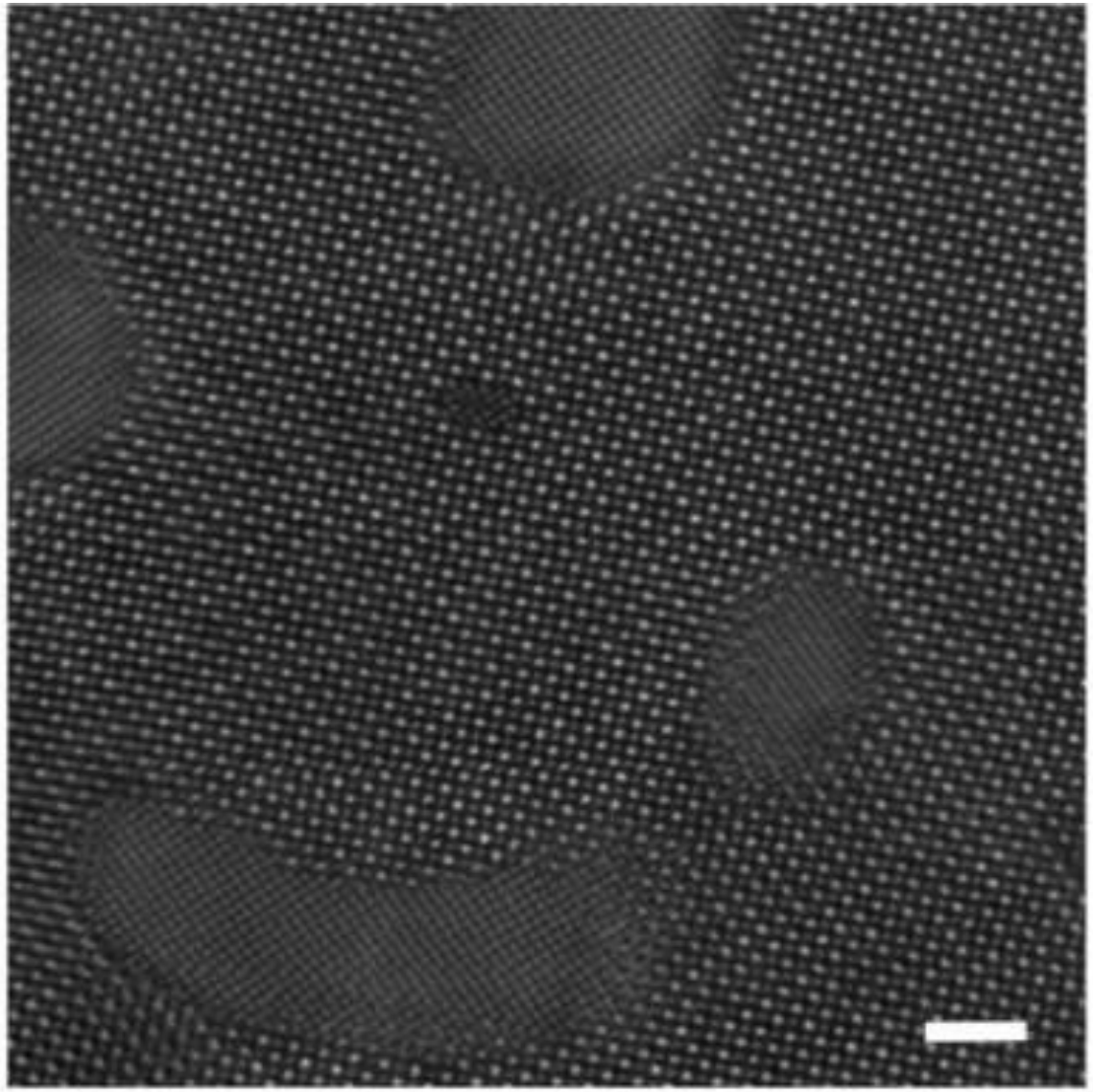


VAE without Atom Finding

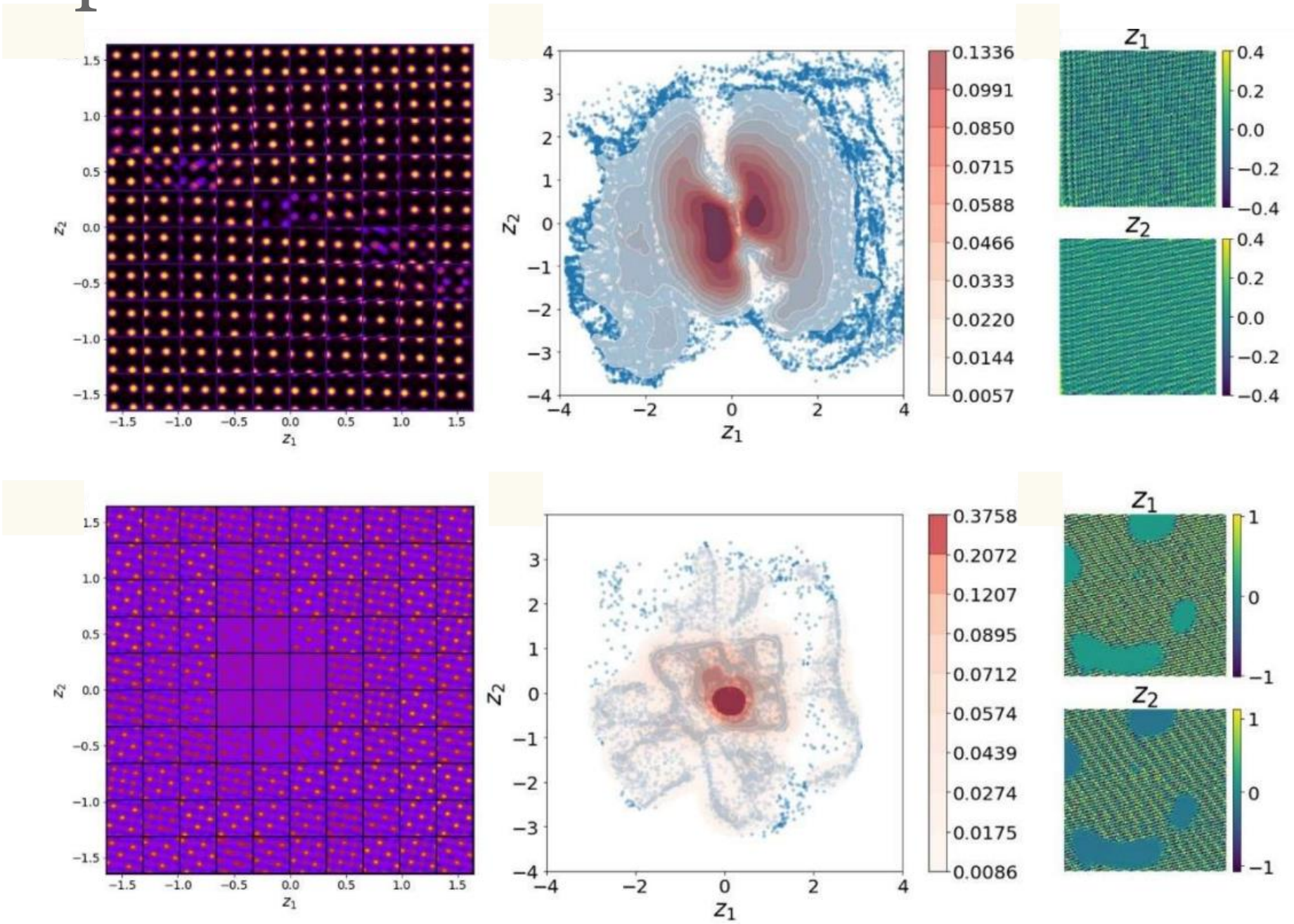
Ferroelectric $BiFeO_3$



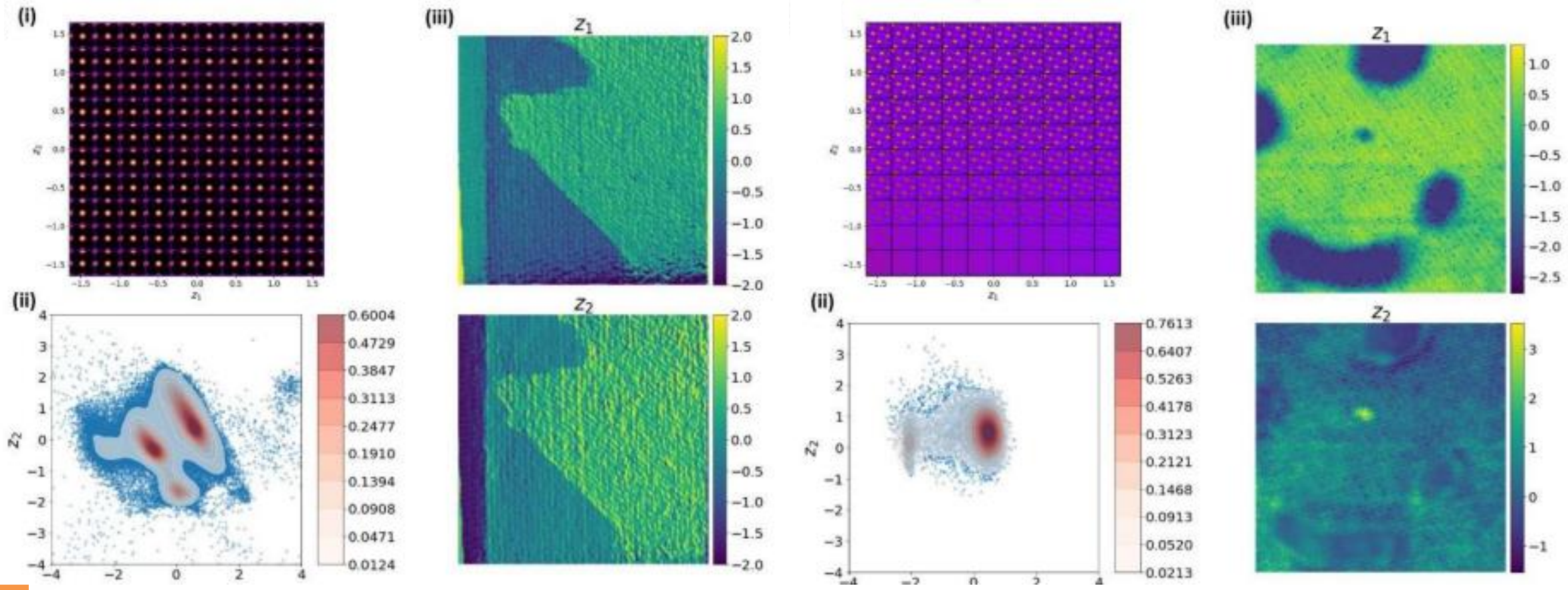
NiO – $La_xSr_{1-x}MnO_3$



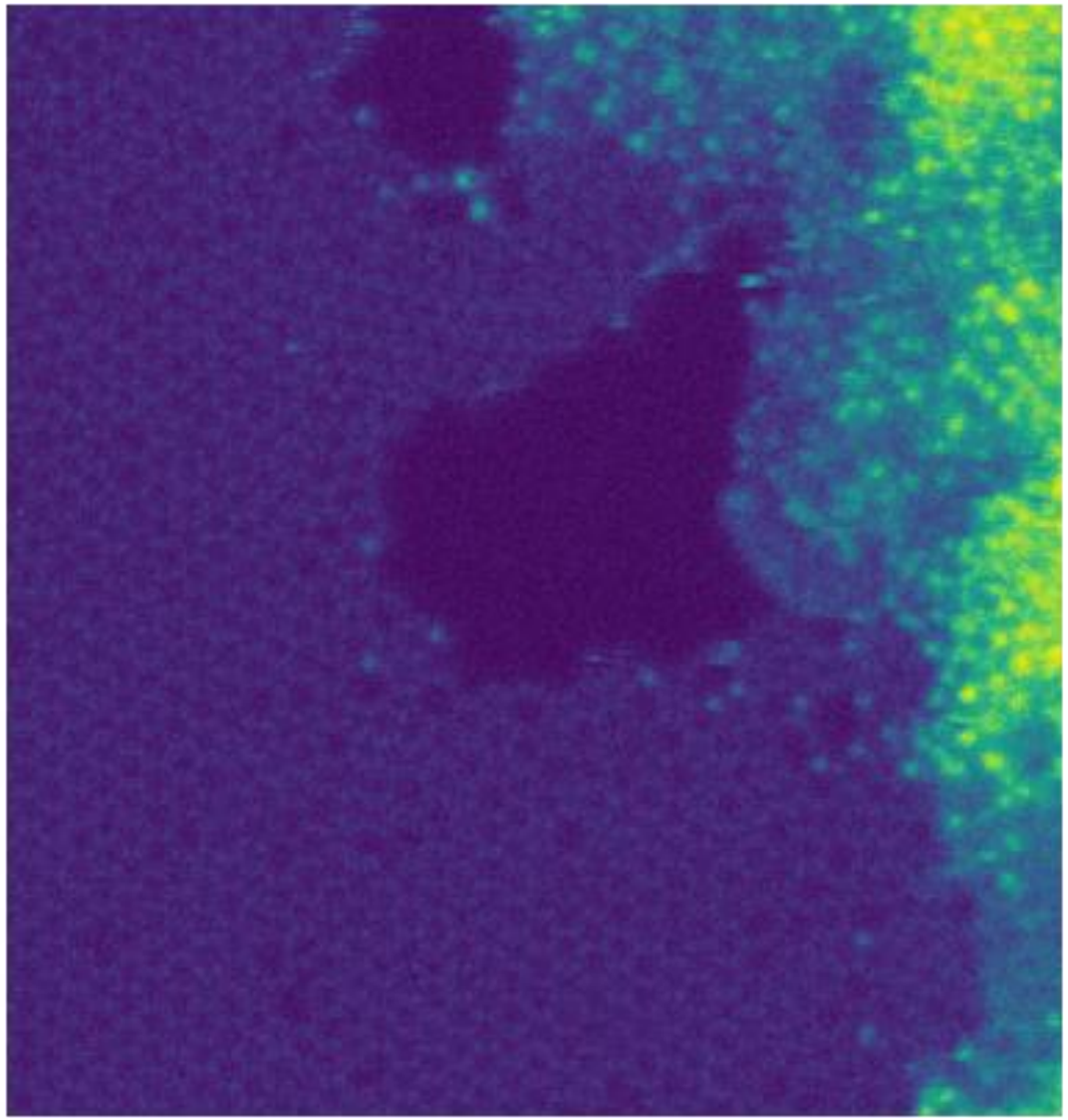
Simple VAE

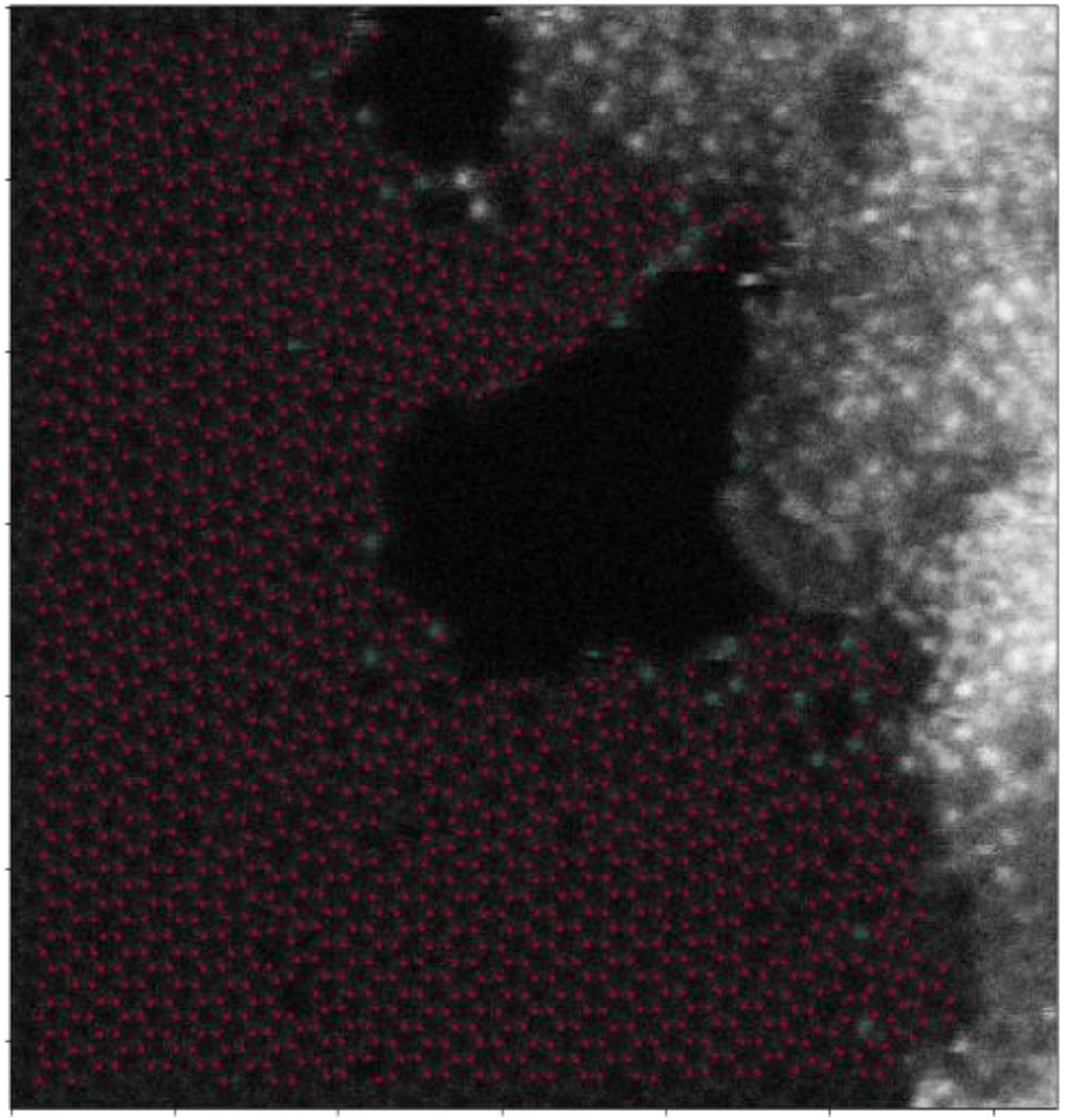

z_1
z_2
0.1336
0.0991
0.0850
0.0715
0.0588
0.0466
0.0333
0.0220
0.0144
0.0057
0.3758
0.2072
0.1207
0.0895
0.0712
0.0574
0.0439
0.0274
0.0175
0.0086

Shift VAE: Translational Invariance

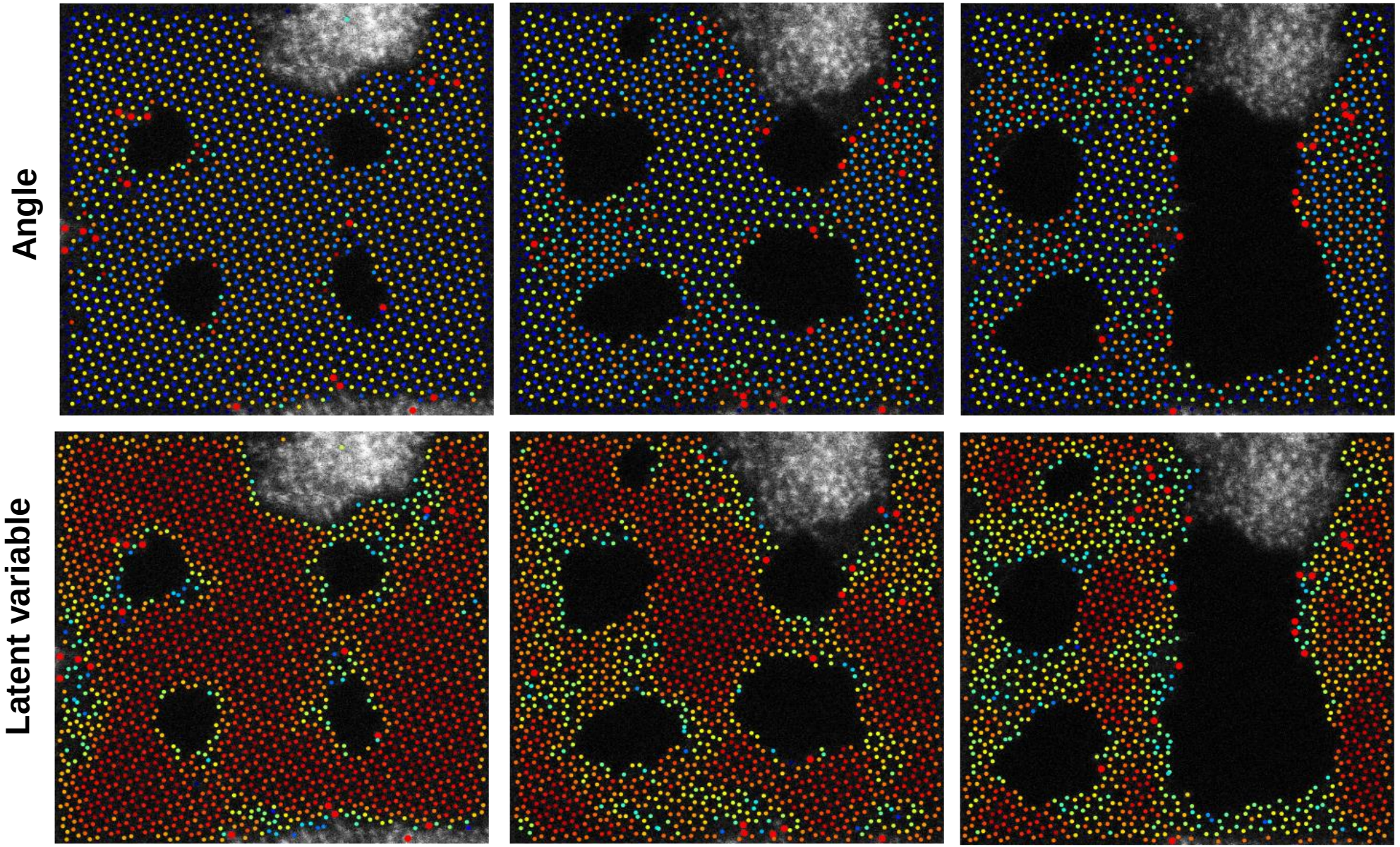


Off to chemically-disordered systems

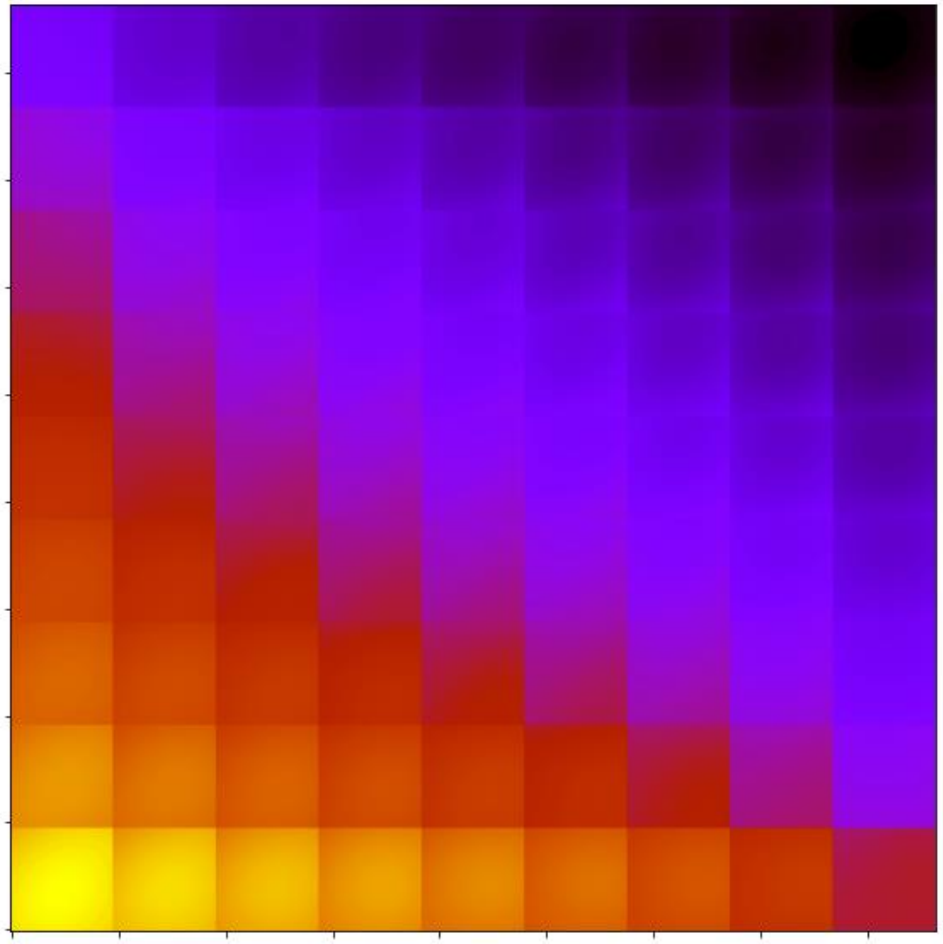


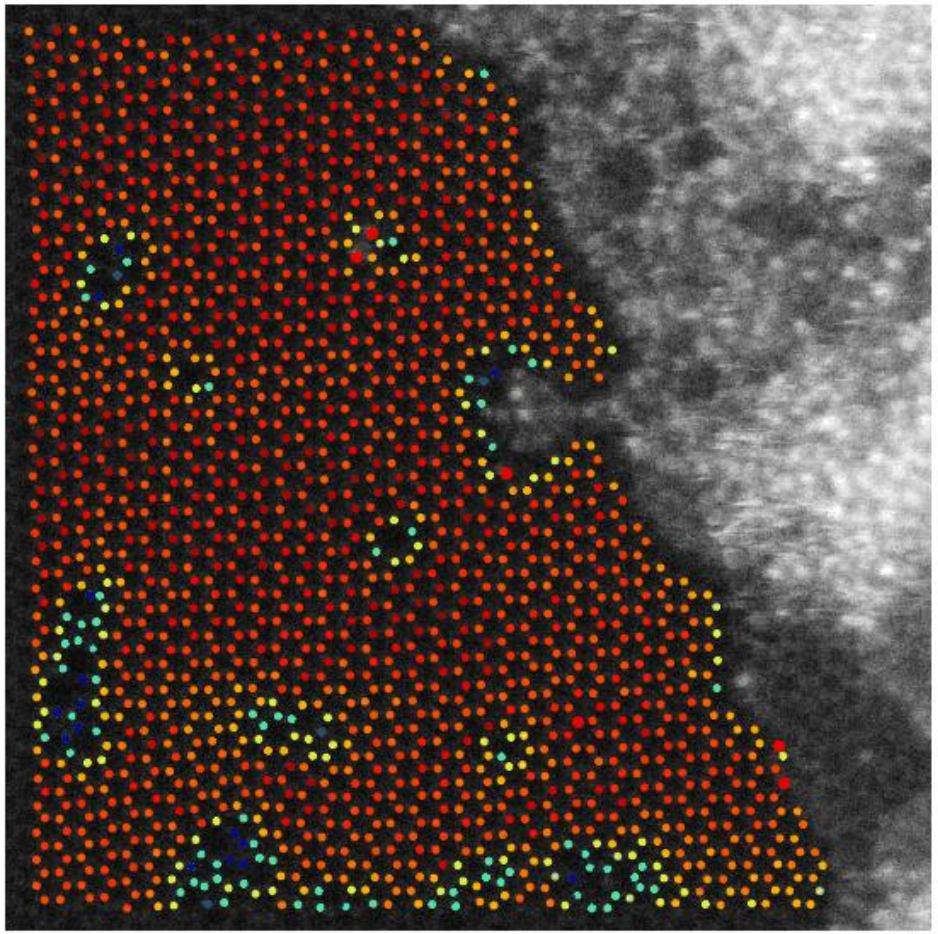


rVAE analysis at different time steps

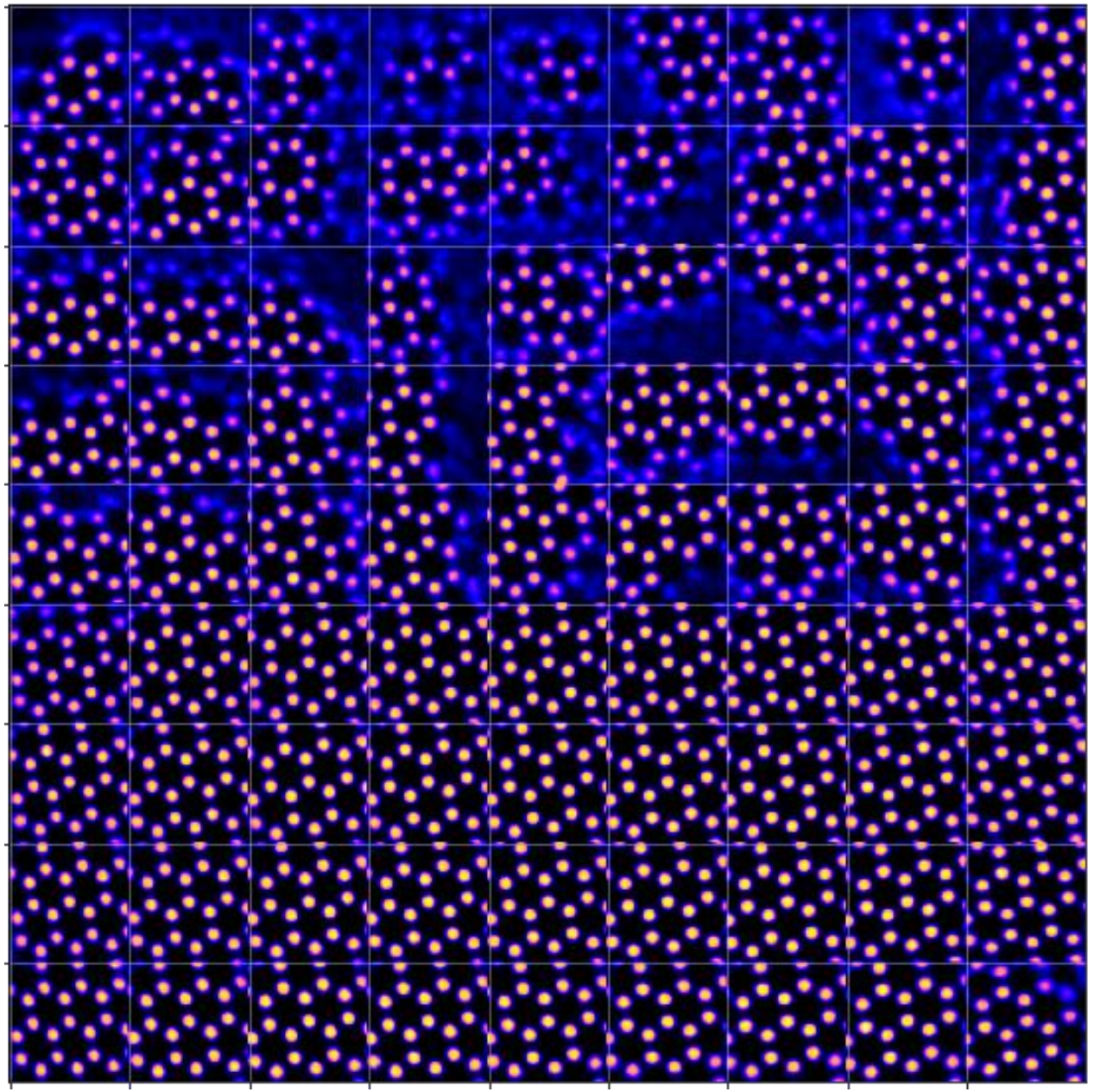


There is nothing as beautiful as training VAE





Next step: skip-rVAE

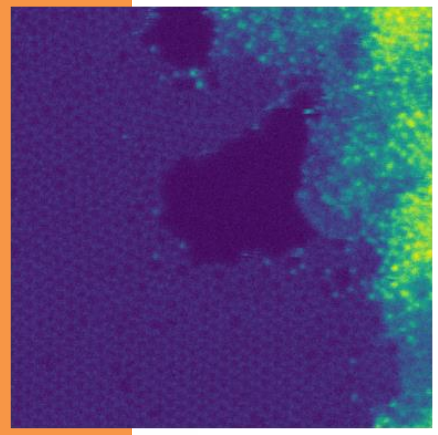


Unsupervised discovery of molecules

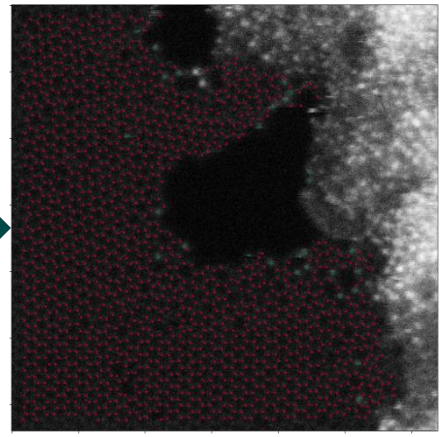
Atom exists, are discrete, and have known shape

Structures are parsimonious in nature

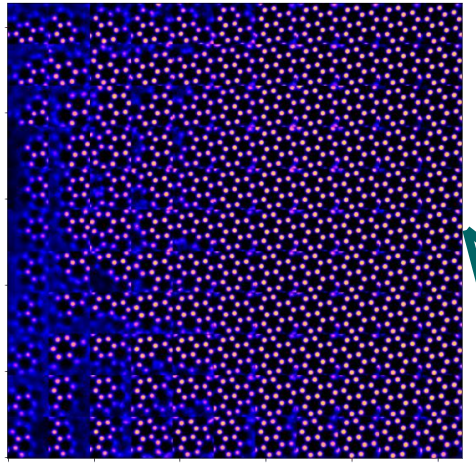
Raw observation



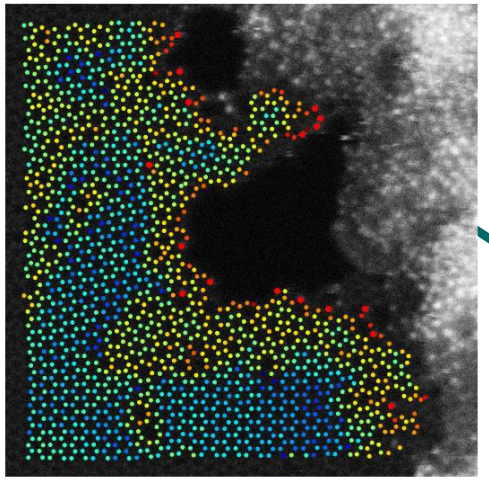
DCNN decoded



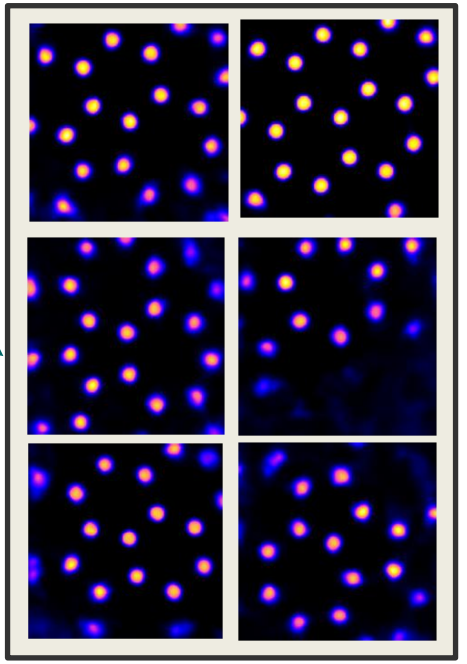
Latent space of srVAE



Latent labels



I. Molecules



II. Reaction networks

A -> B -> C

Exploring the latent space structure