THE UNIVERSITY of TENNESSEE KNOXVILLE

Lecture 36: Encoder-decoders and Dual VAEs

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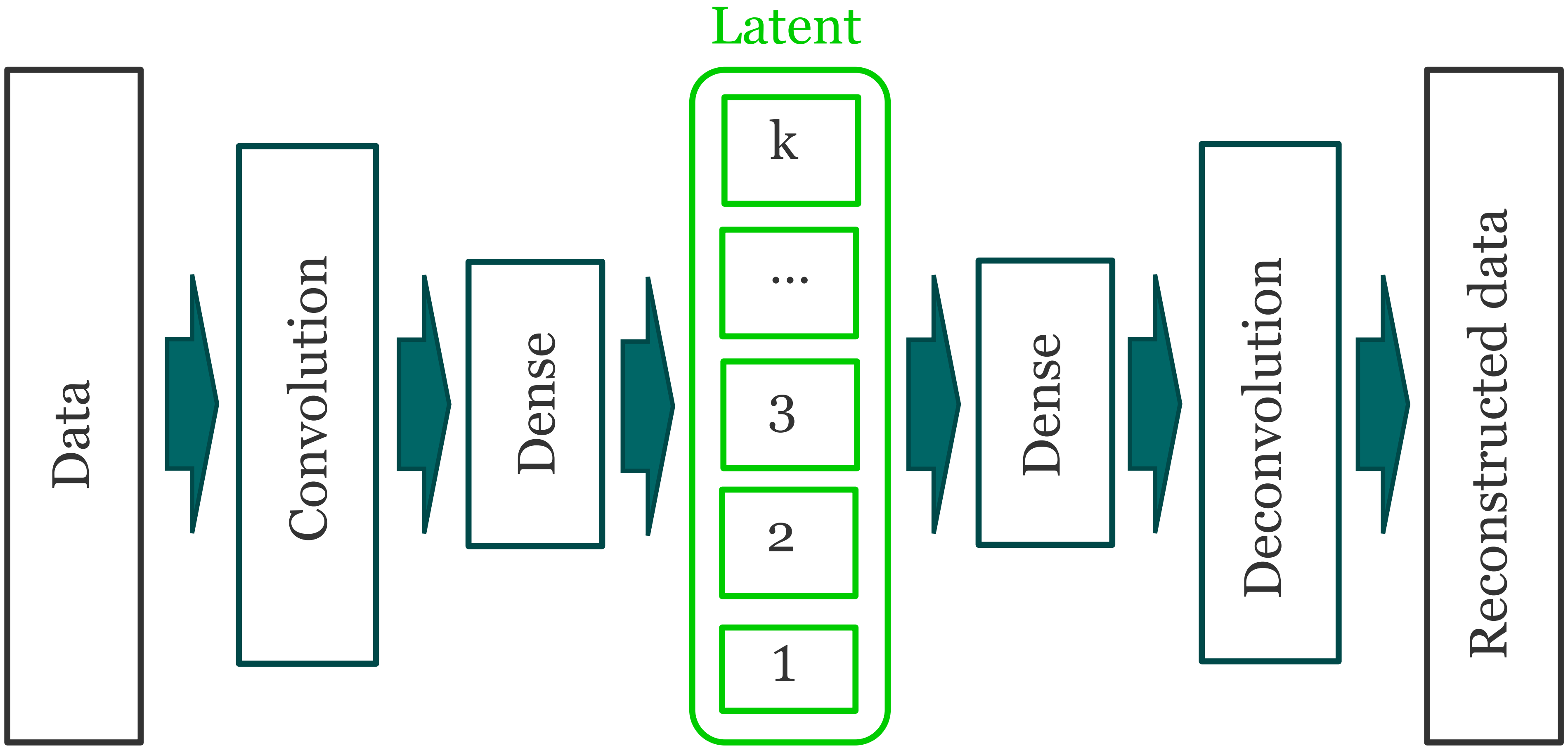
Autoencoders



Loss: (some form of) reconstruction loss

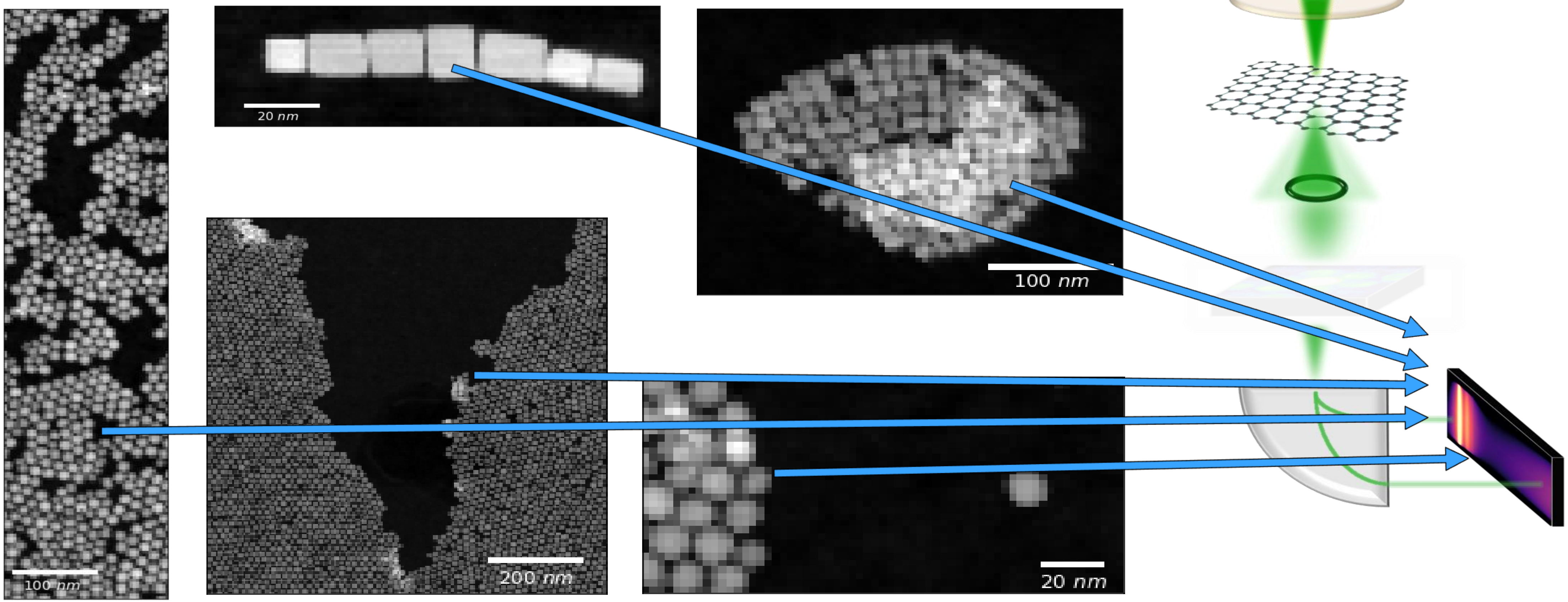
Do we have to encode and decode the same type of objects?

Examples of structure property relationships

- Molecular structure – optical spectroscopy
- Atomic configurations in catalysts – catalytic activity
- Protein sequence – geometry
- Photonic structure – optical adsorption
- Materials microstructure – dielectric/conductive properties
- Composite structure – electrochemical properties
- Antenna shape – emission characteristics
- … and many more

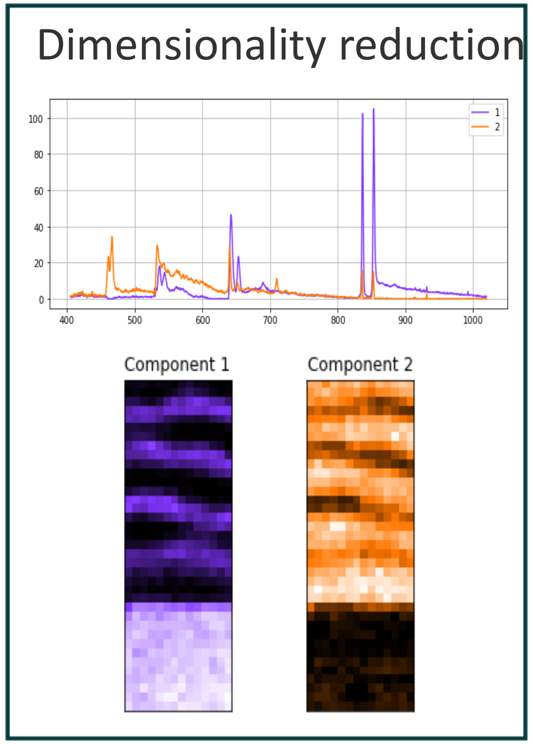
Practical Use Case: EELS

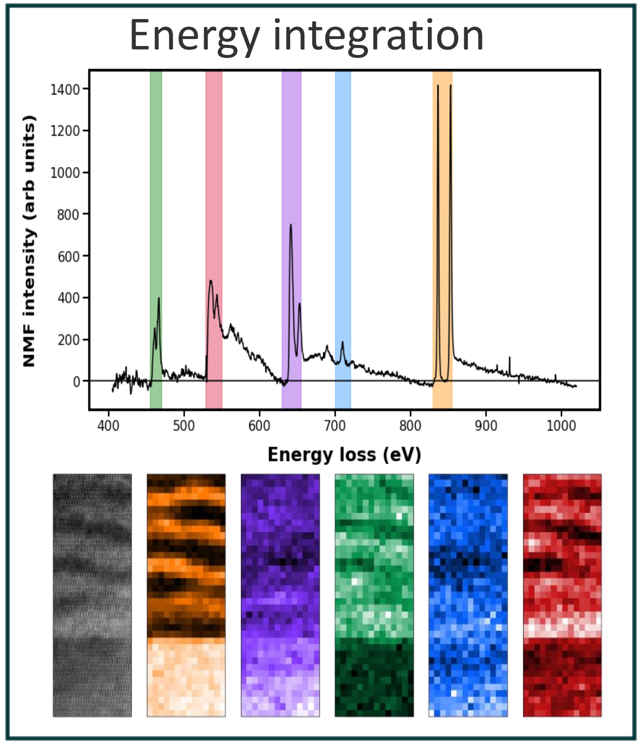
- Self-assembled monolayer of **metal oxide nanoparticles** (**F**,**Sn** co-doped indium oxide)
- **Sn** tunes the plasmon resonance by supply of additional e^- (F concentration fixed)
- Variety of geometric configurations also present

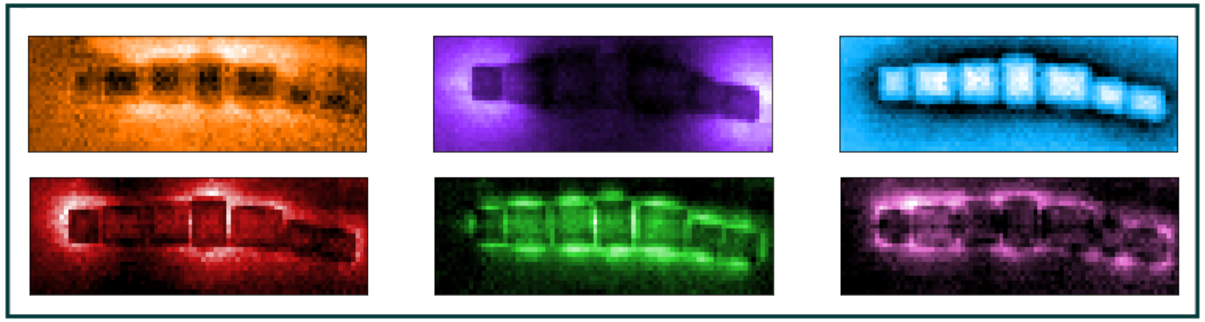


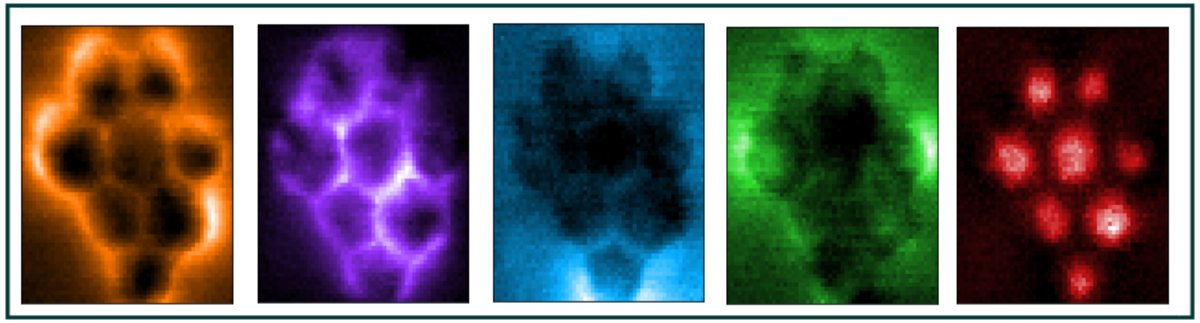
EELS

- Can consider to be another signal in the form of a **1D spectrum**
- Collect EEL spectrum in an (x,y) grid: EELS imaging
- To better visualize / understand these 3D signals, can integrate specific spectral bands, or dimensionally reduce (PCA, NMF) them
- Applications in plasmonics & nanophotonics

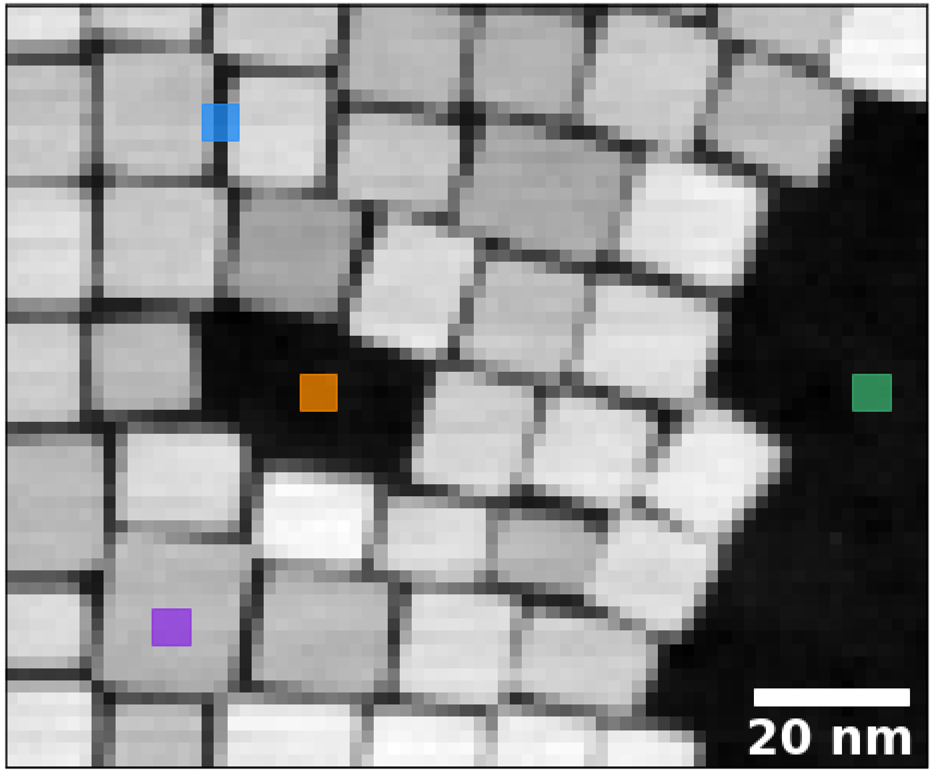


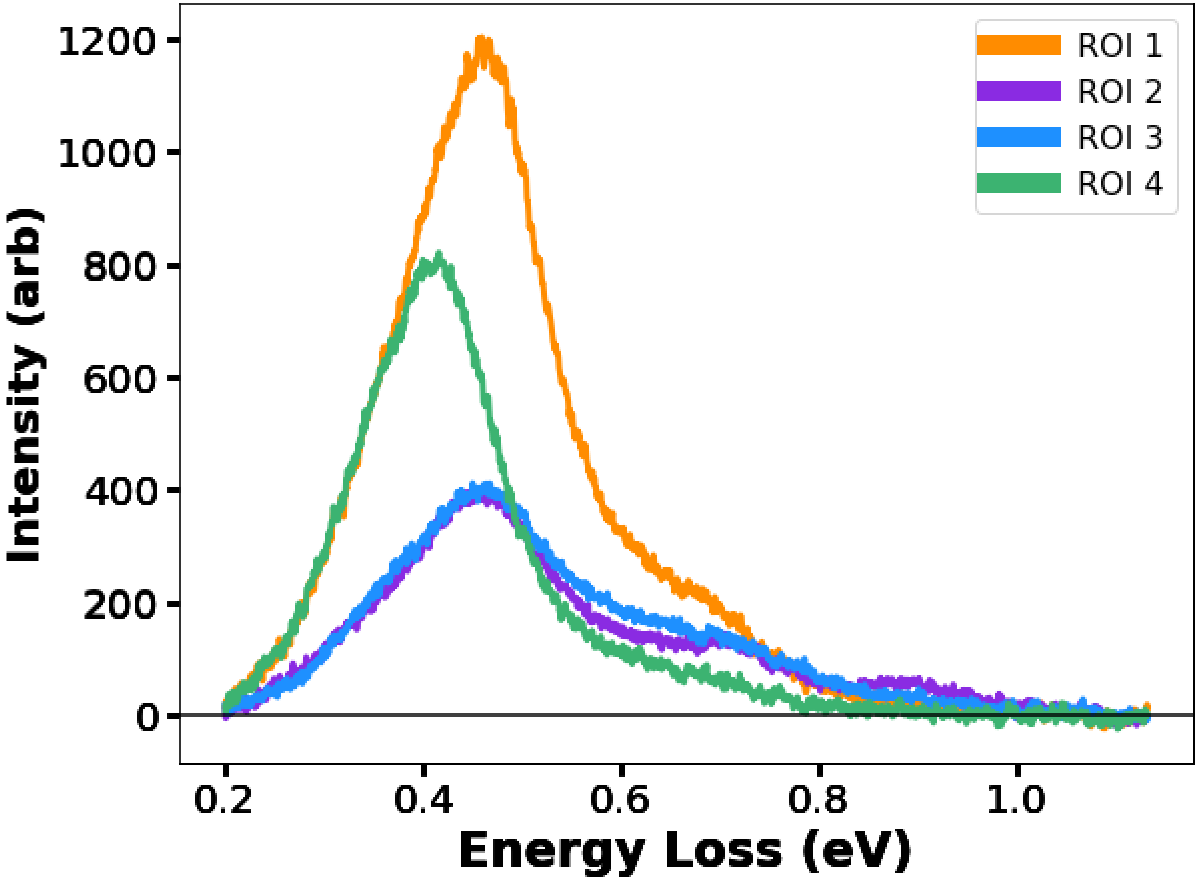






But what about the structure-property relations?

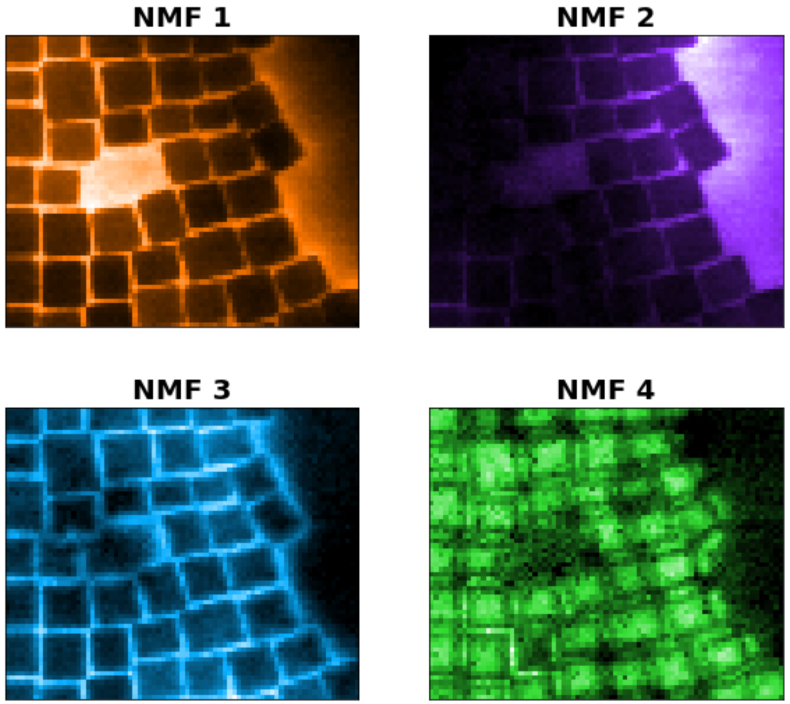


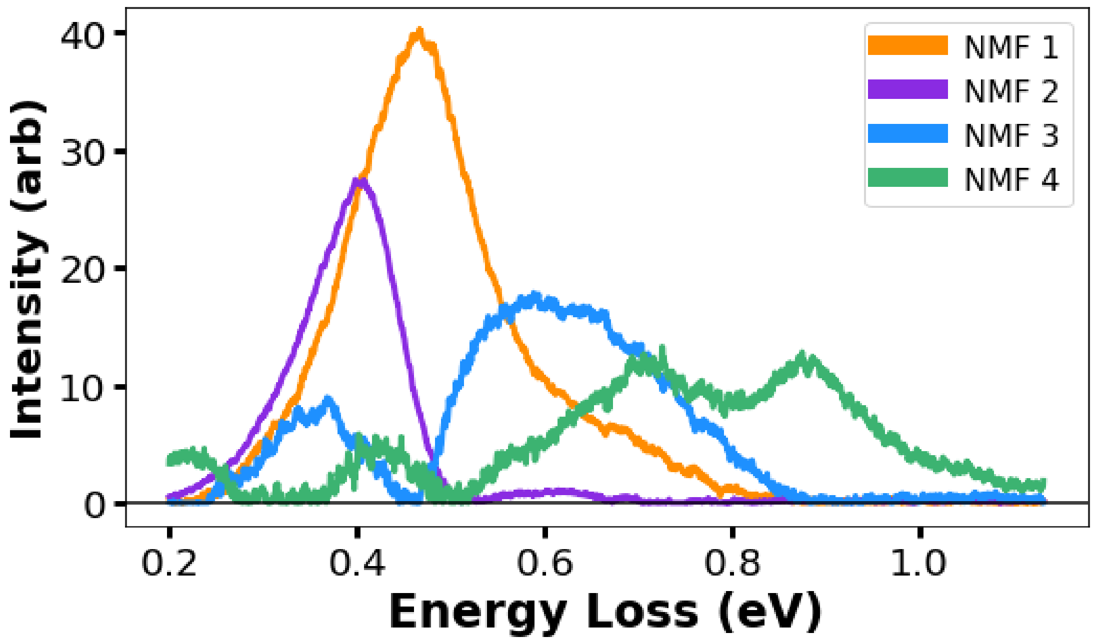


By inspection, we can note some characteristic aspects of spectra from specific types of geometries. However:

- How can we prove it and quantify this relationship?
- How universal is it for similar structures?
- Can we discover structures that will have the properties that we want?

Exploratory data analysis

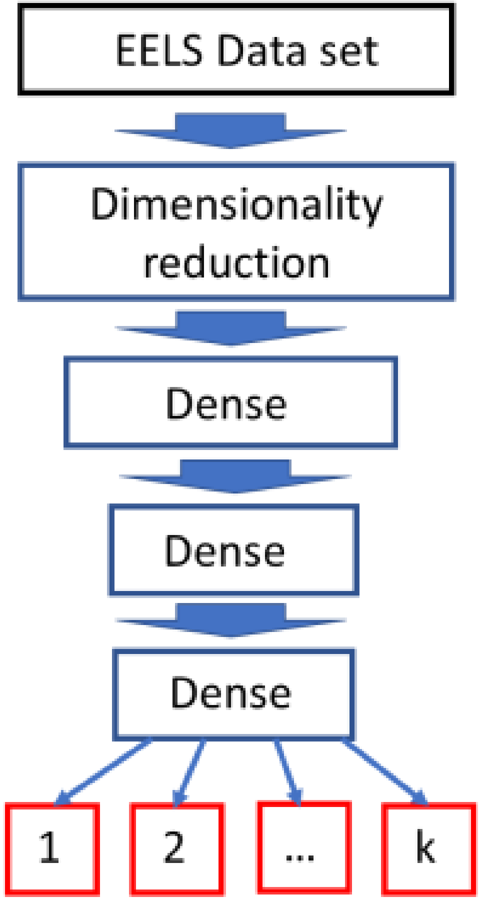


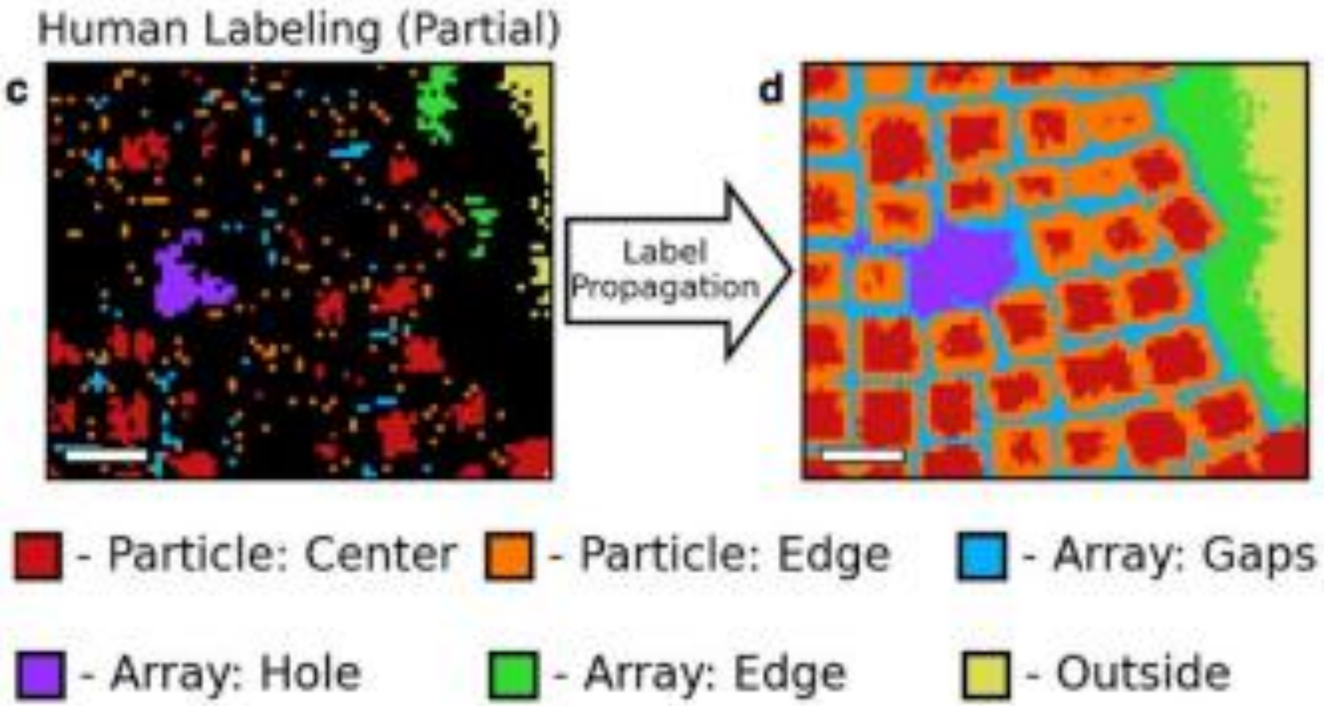


- Great way to explore system
- Visualization of hyperspectral data

- Multiple modes per pixel
- Non-physical extraction
- No relationship with geometry established

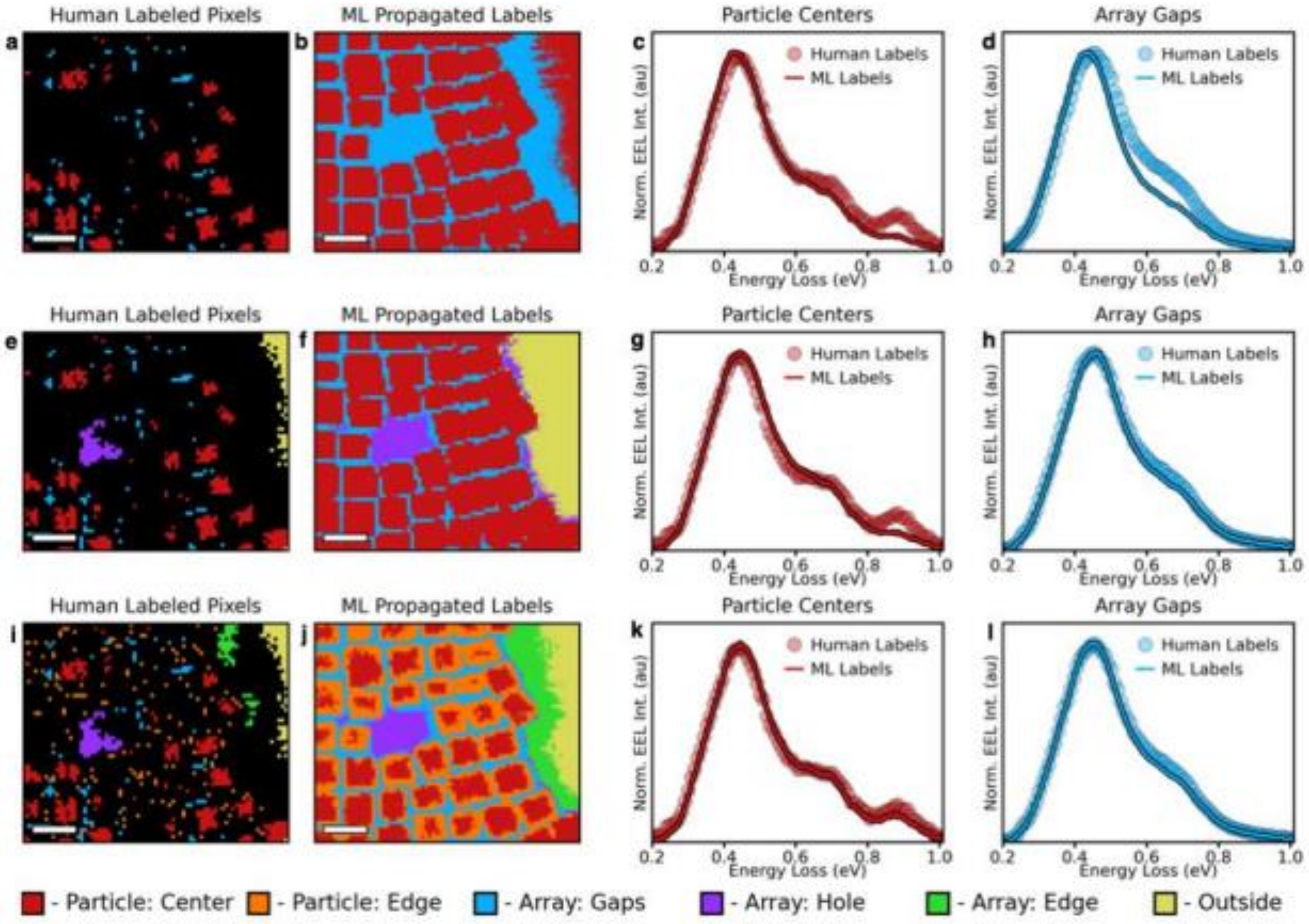
Strategy 1: Labelling





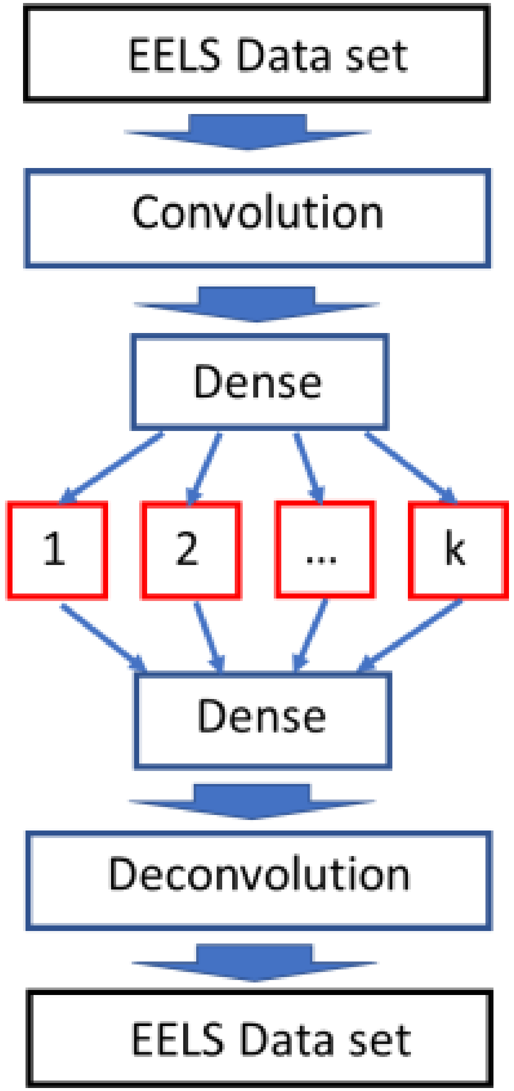
- Define attributes by semi-manual inspection
- Create training data set
- Train the classifier
- Apply the classifier to the remainder of the data set

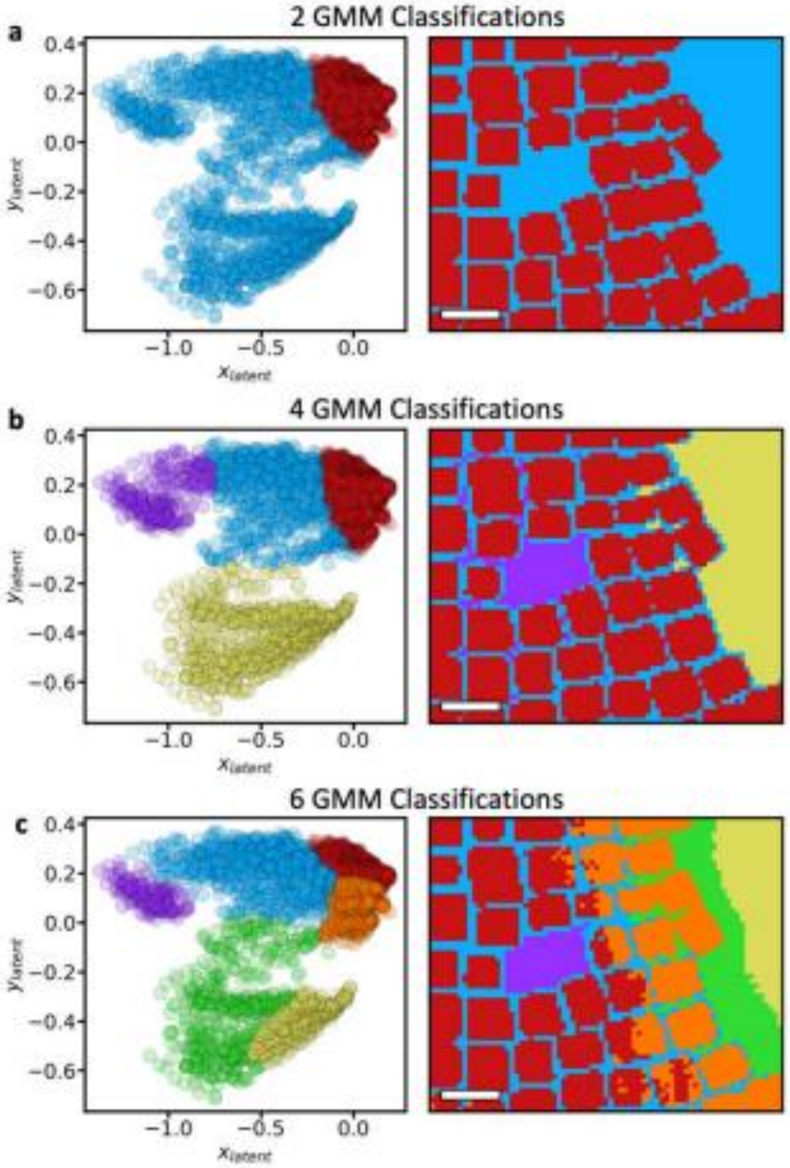
Strategy 1: Labelling



- Problem: human labels can be ambiguous

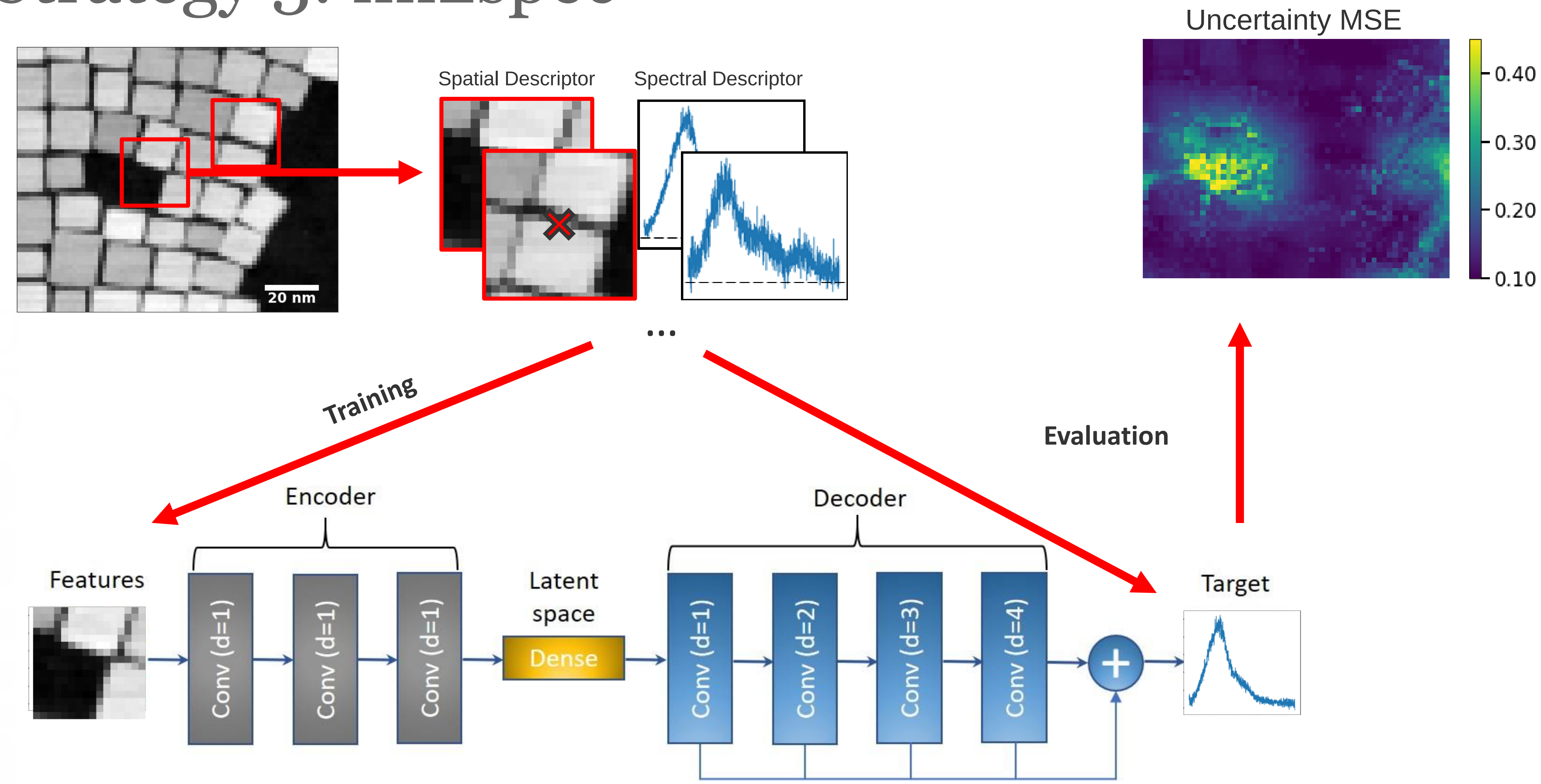
Strategy 2: AE Labels





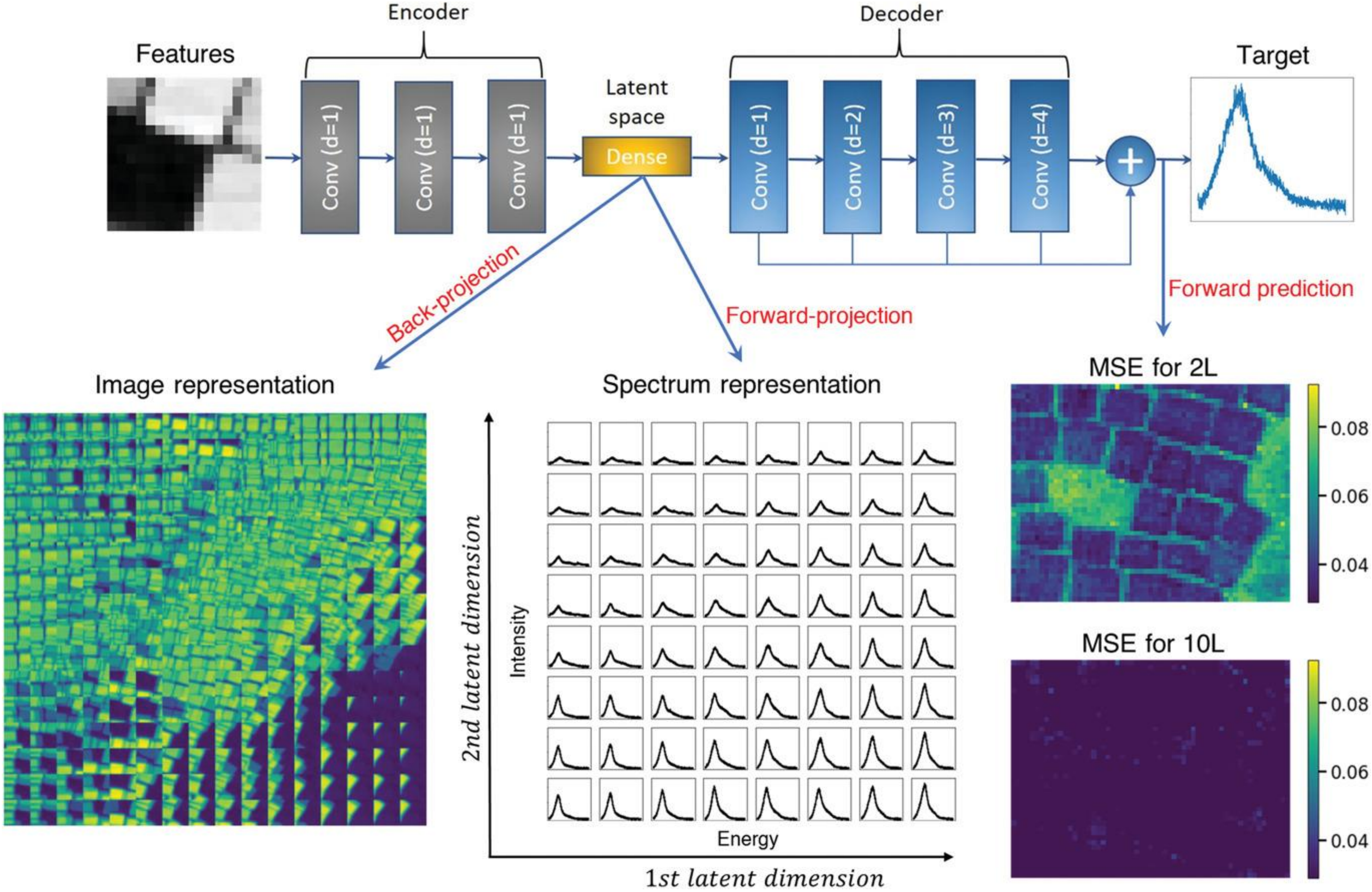
- Unsupervised learning on spectral data: we make conclusions based on maps

Strategy 3: im2spec

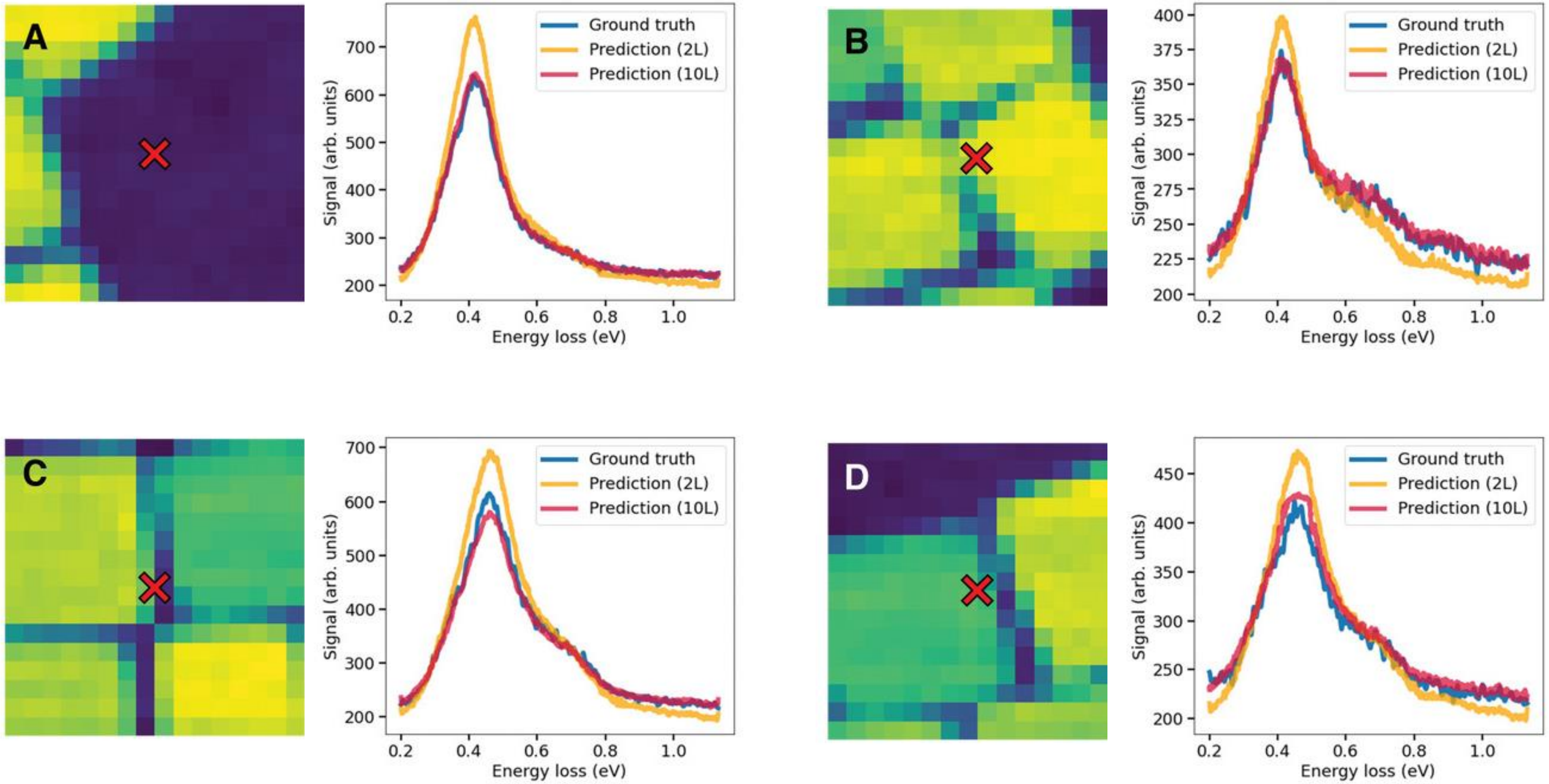


What if we create a network that encodes structure, and decodes spectra?

Im2spec: latent space visualization

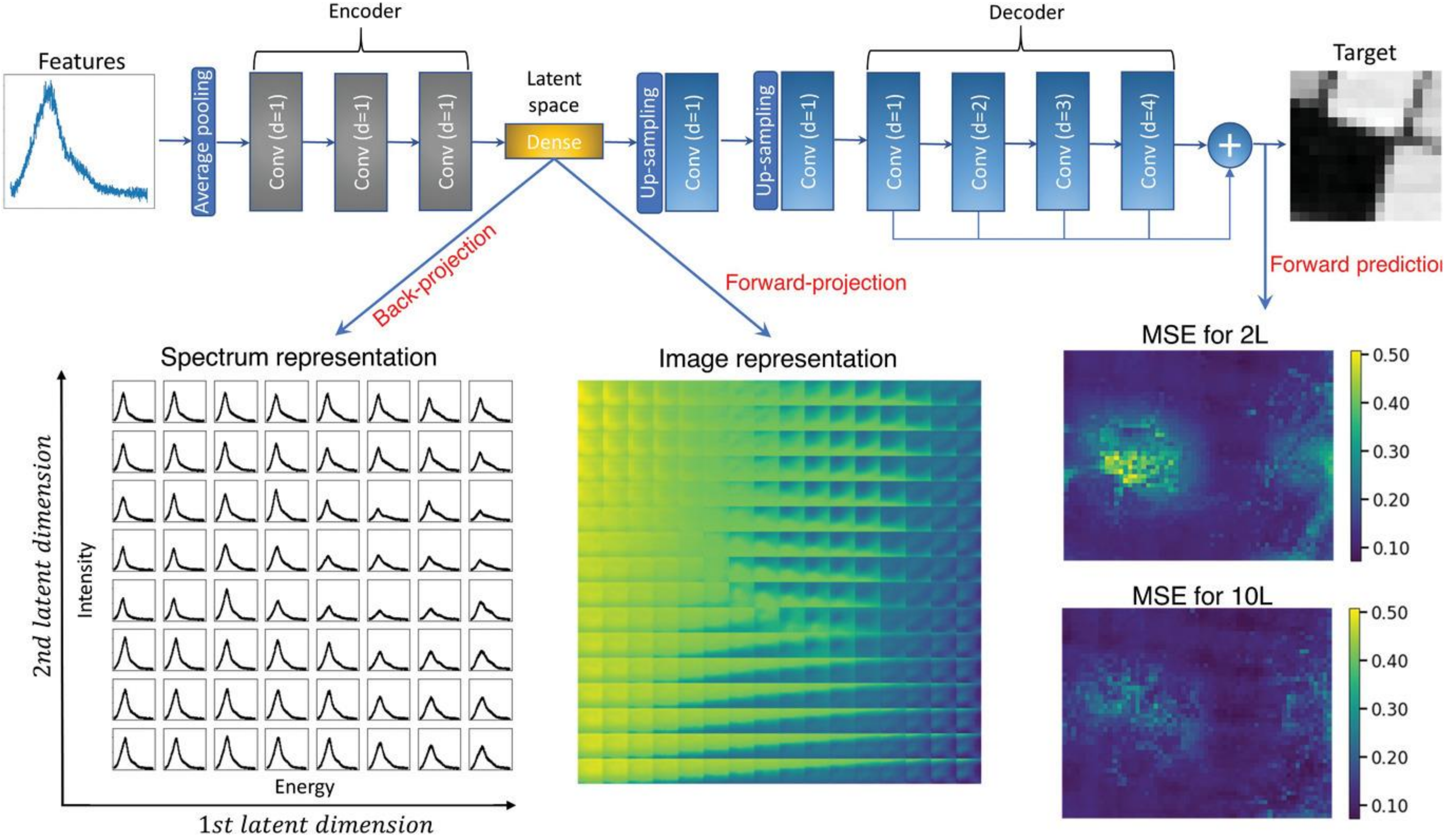


Im2spec prediction



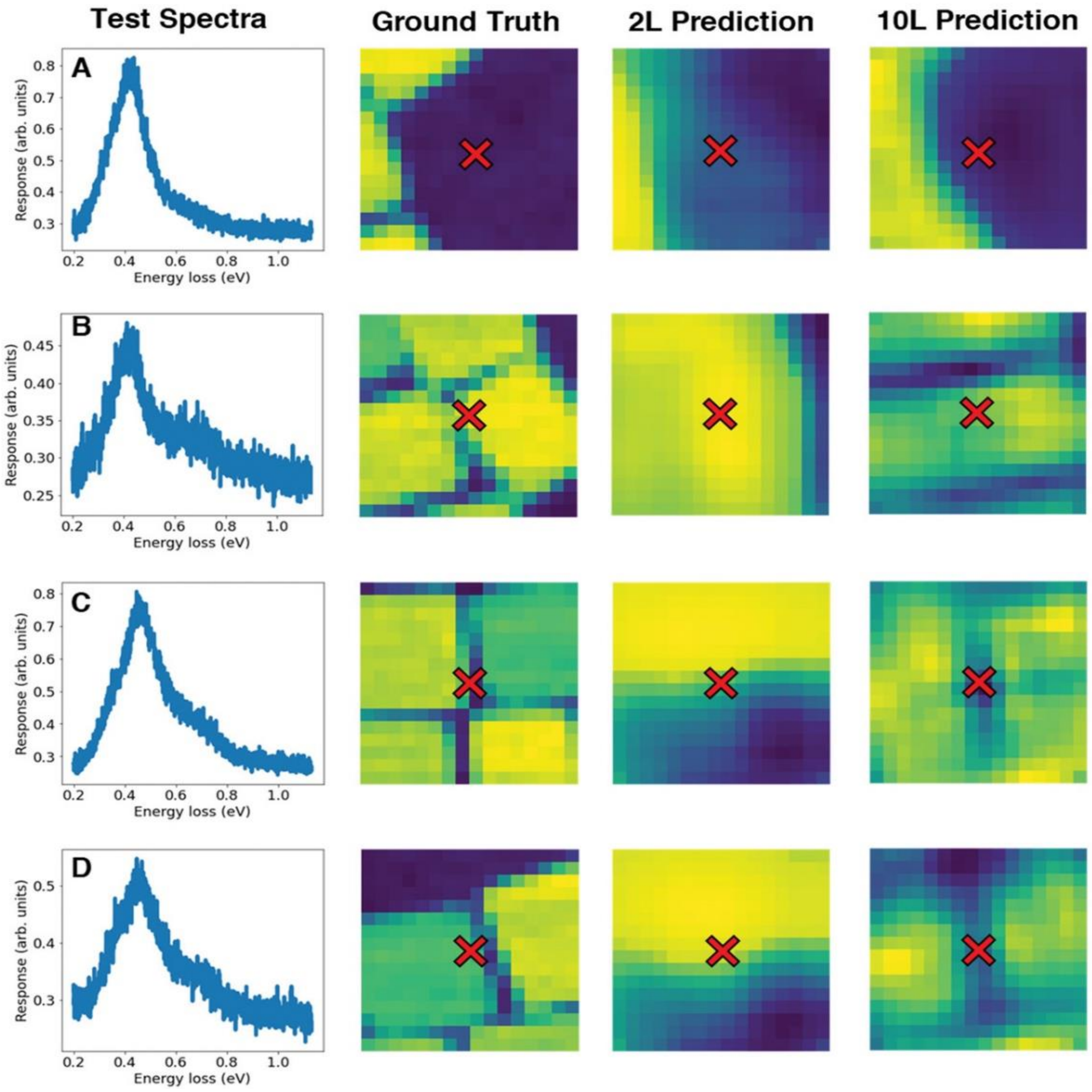
- After training, predict the spectral response of a geometric arrangement that the network has **never encountered**
- **Library** of geometric-plasmonic relationships
- Can be used for solution of inverse design in nanophotonics and other fields

Spec2im



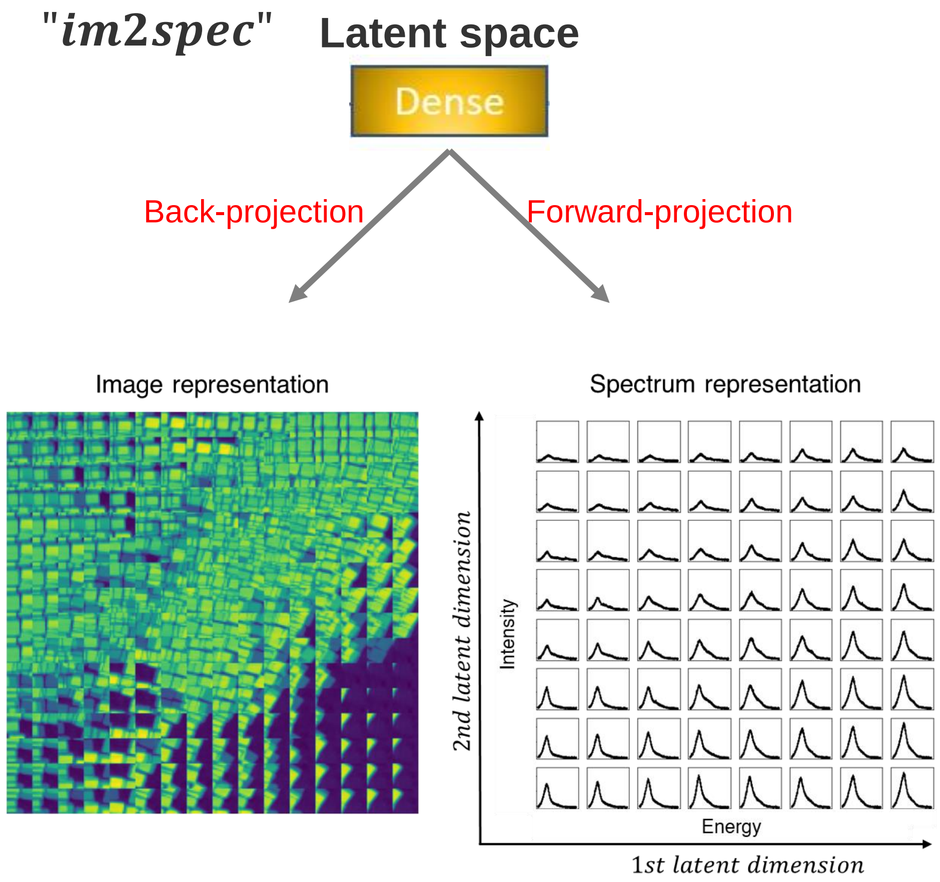
Encoder
Decoder
Features
Average pooling
Conv (d=1)
Conv (d=1)
Conv (d=1)
Latent space
Dense
Up-sampling
Conv (d=1)
Up-sampling
Conv (d=1)
Conv (d=1)
Conv (d=2)
Conv (d=3)
Conv (d=4)
Target
Back-projection
Forward-projection
Forward predictio
Spectrum representation
Image representation
MSE for 2L
MSE for 10L
2nd latent dimension
Intensity
Energy
1st latent dimension
0.50
0.40
0.30
0.20
0.10

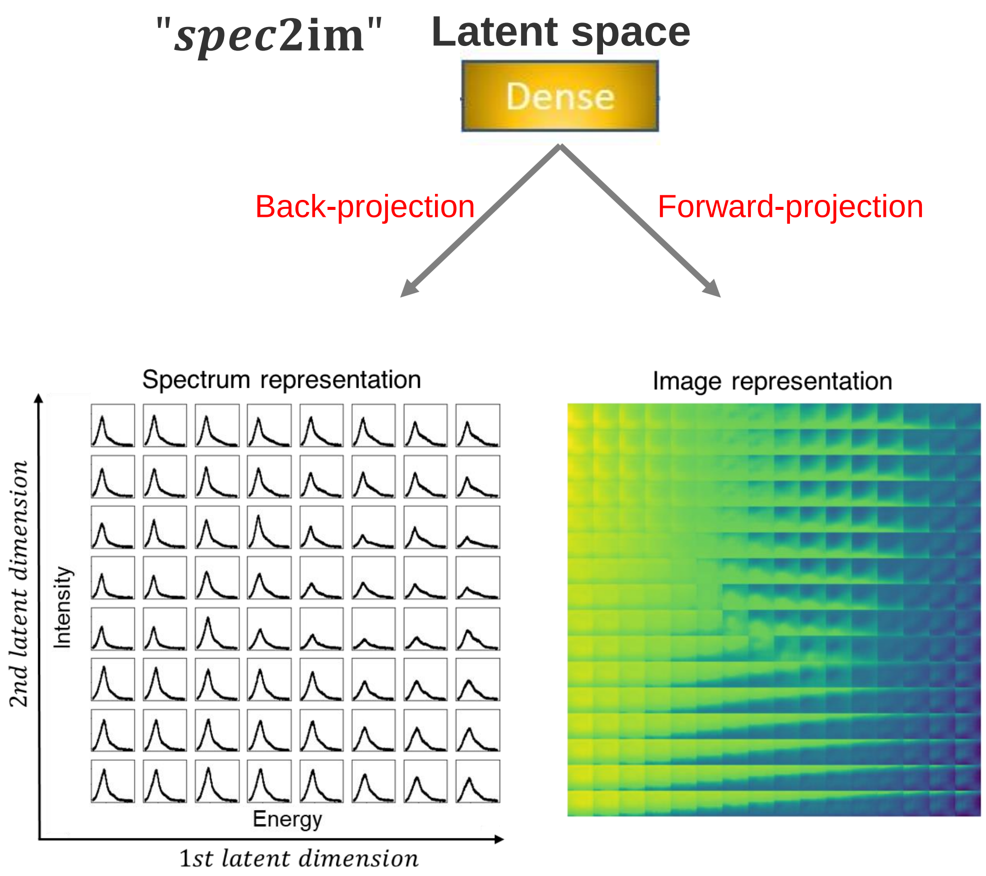
Spec2im predictions



- After training, predict the spectral response of a geometric arrangement that the network has **never encountered**
- **2L** and **10L** refers to number of latent dimensions chosen

Spec2im and im2spec

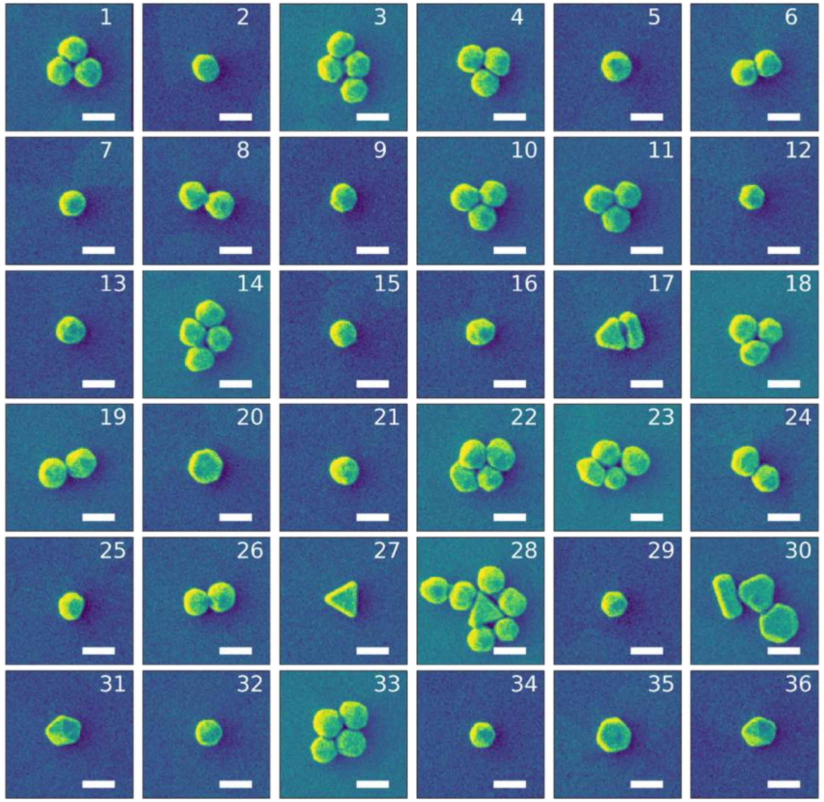




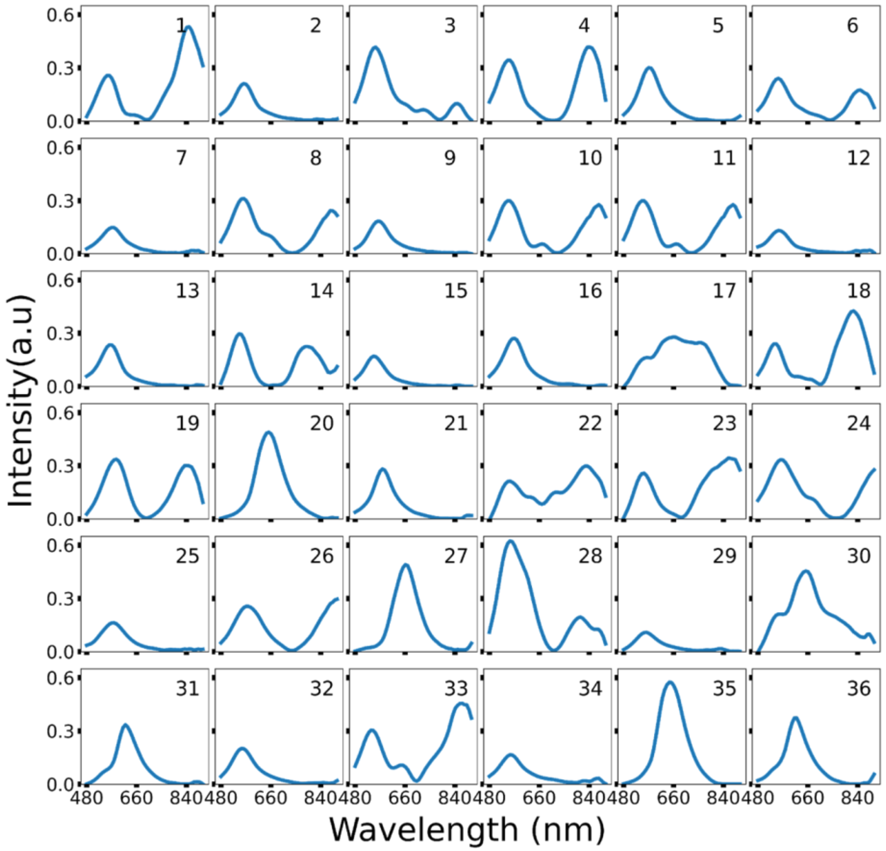
- Problem with im2spec and spec2im: they are generative only wrt. one transformation

Dual VAE: structure-property relationships

SEM images: "Structure Information"

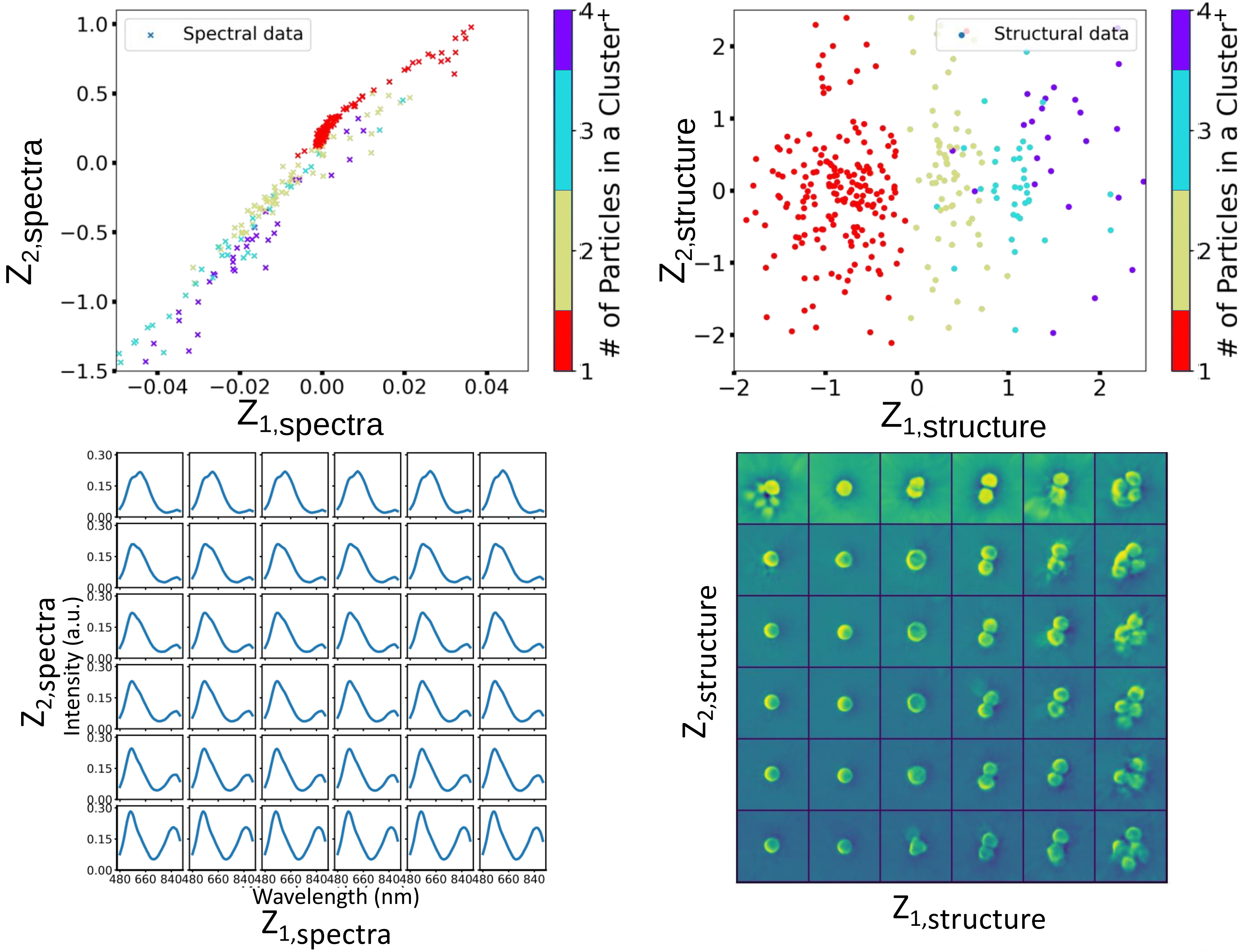


Hyperspectral microscope: "Property Information"

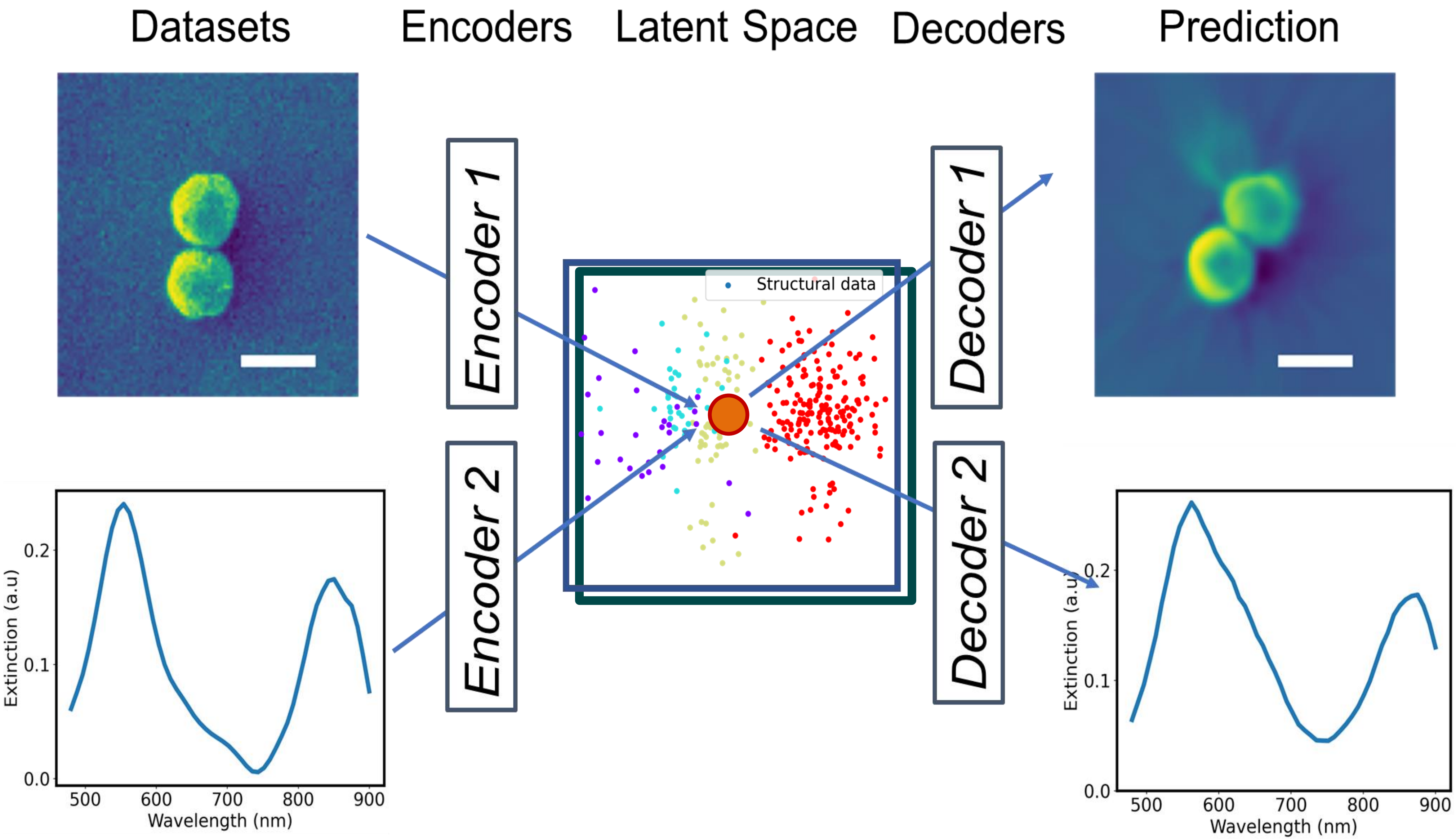


- Far field optical spectroscopy: images and spectra
- Here, we also have simple labels (number of clusters)

Separated VAE



Dual VAE

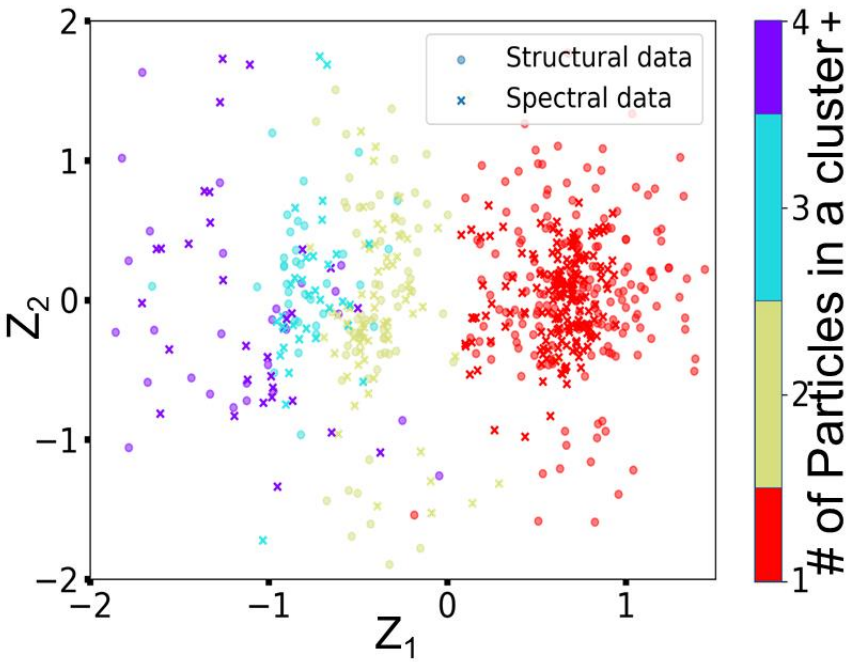


Datasets
Encoders
Latent Space
Decoders
Prediction
Encoder 1
Encoder 2
Structural data
Decoder 1
Decoder 2
Extinction (a.u)
0.0
0.1
0.2
500
600
700
800
900
Wavelength (nm)

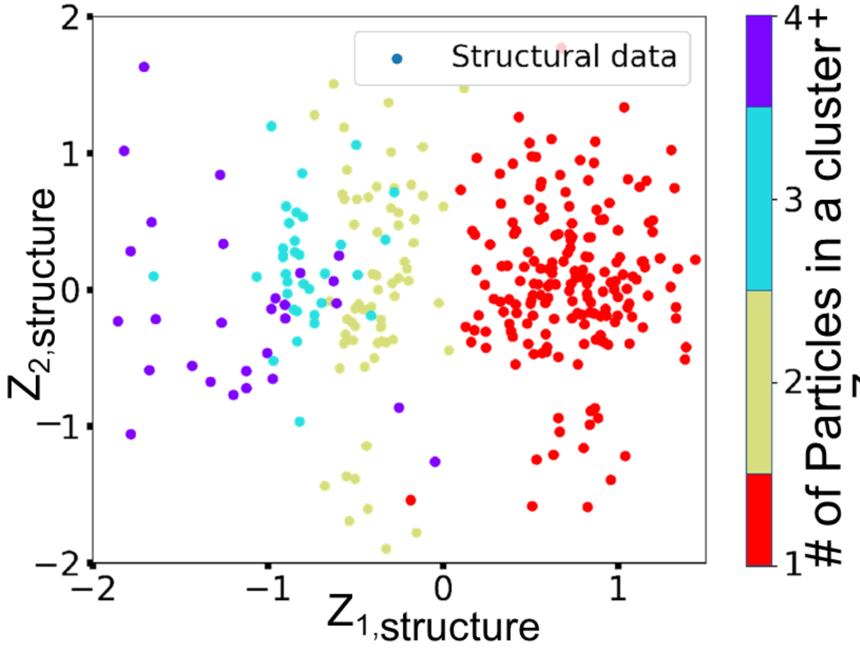
Dual VAE: Latent Distributions

Latent Space Representation

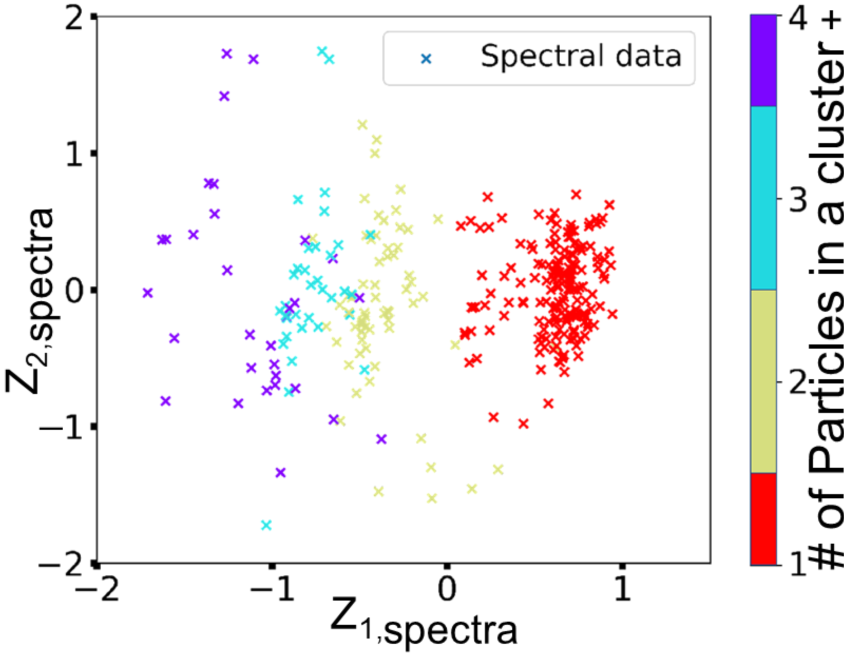
“Dual Latent Space”



“Structure Information”

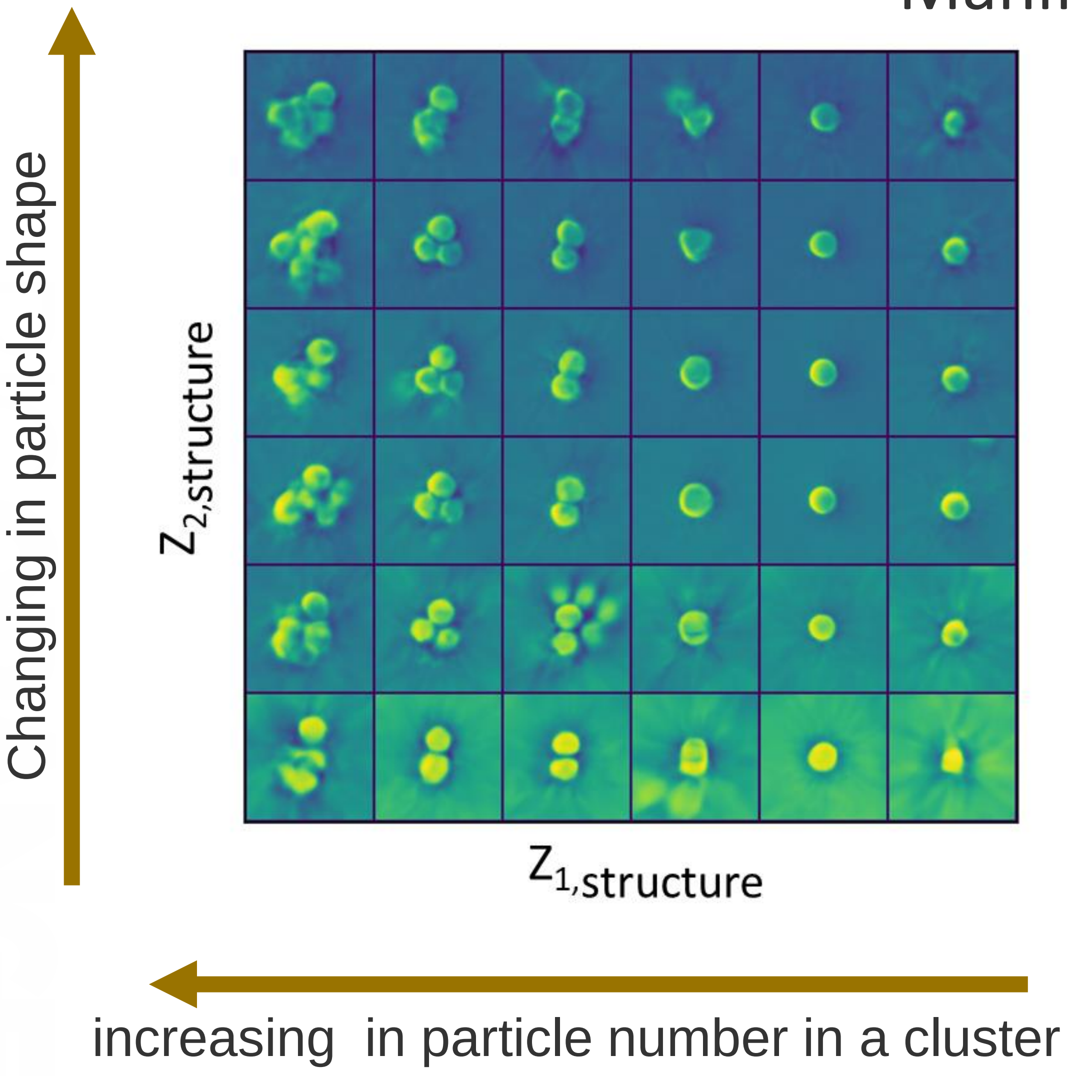


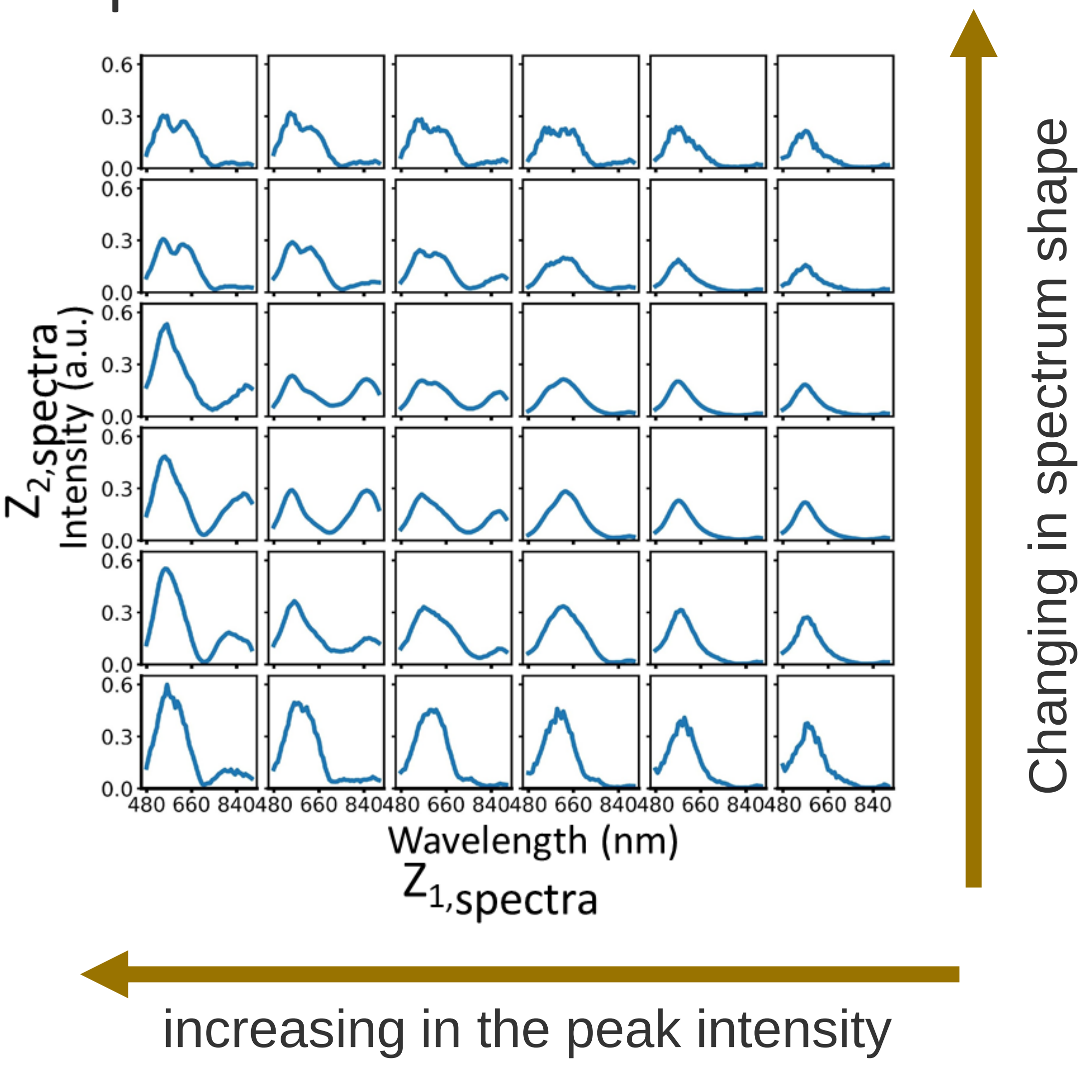
“Property Information”



Dual VAE: Latent Representations

Manifold Representation





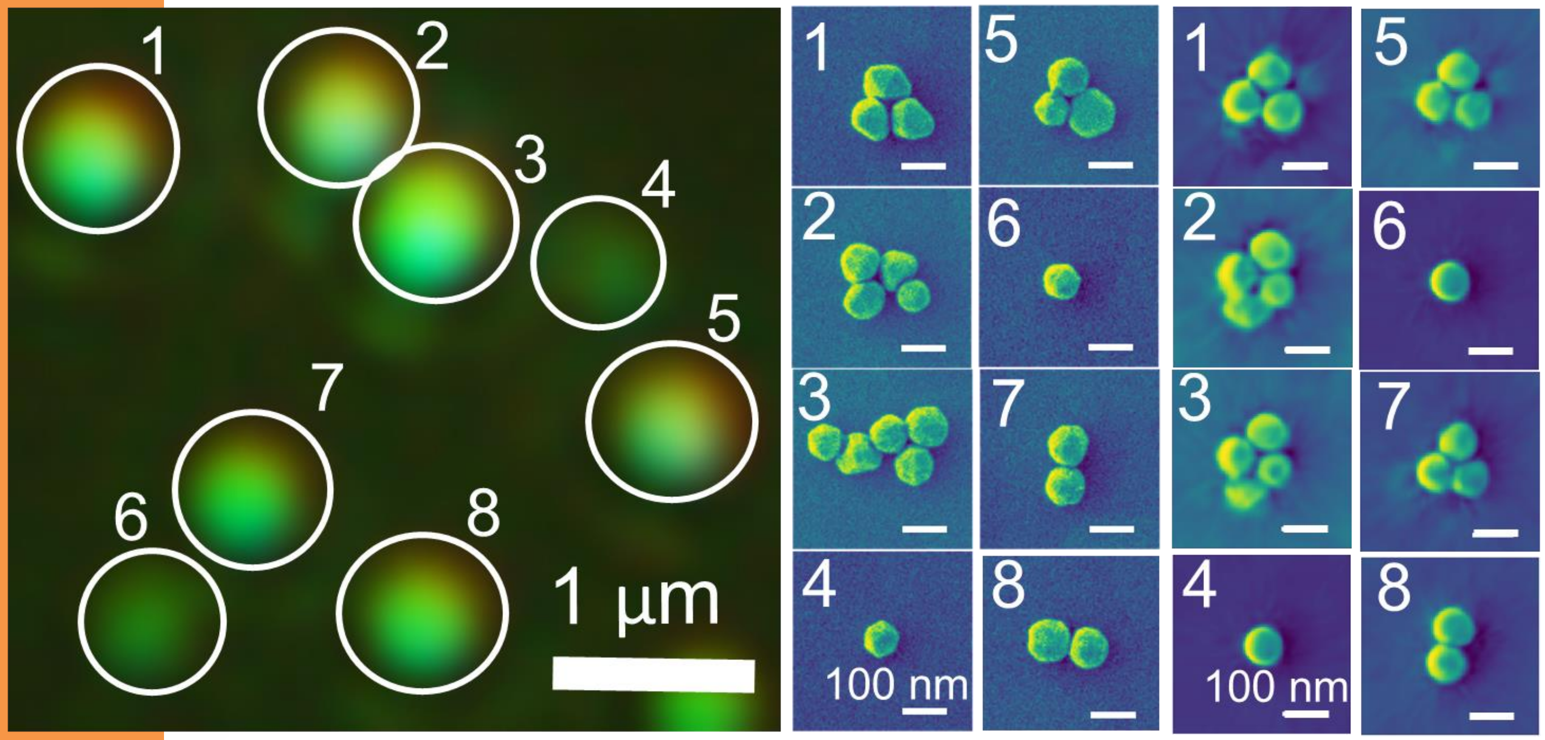
Dual VAE: Predictions

Example

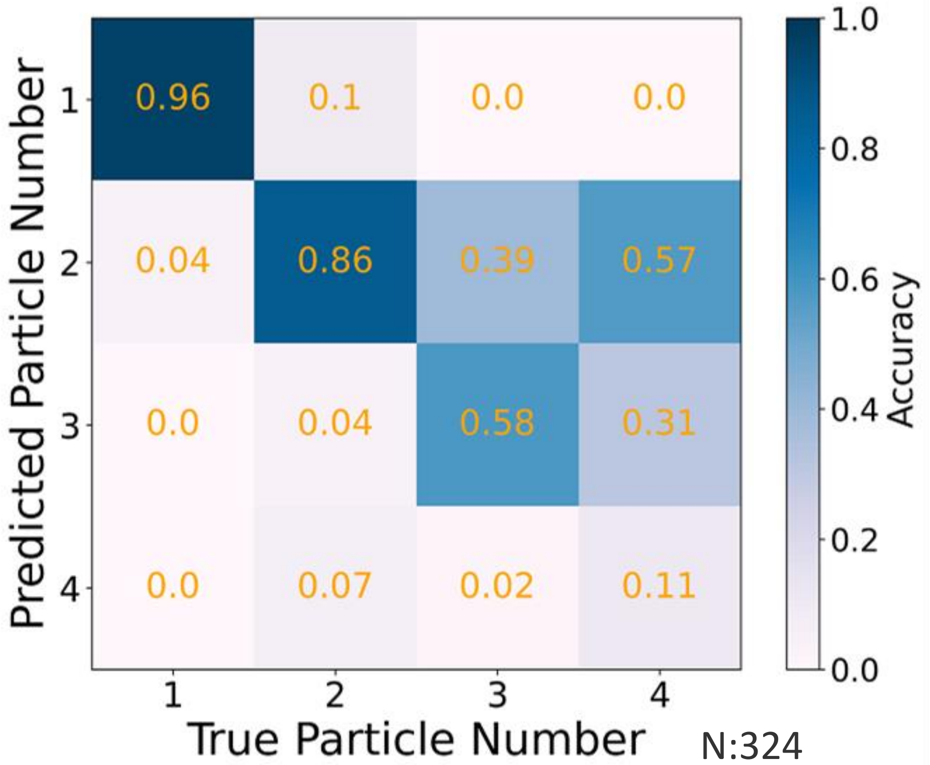
Darkfield Image

Ground Truth

Prediction



Overall Particles



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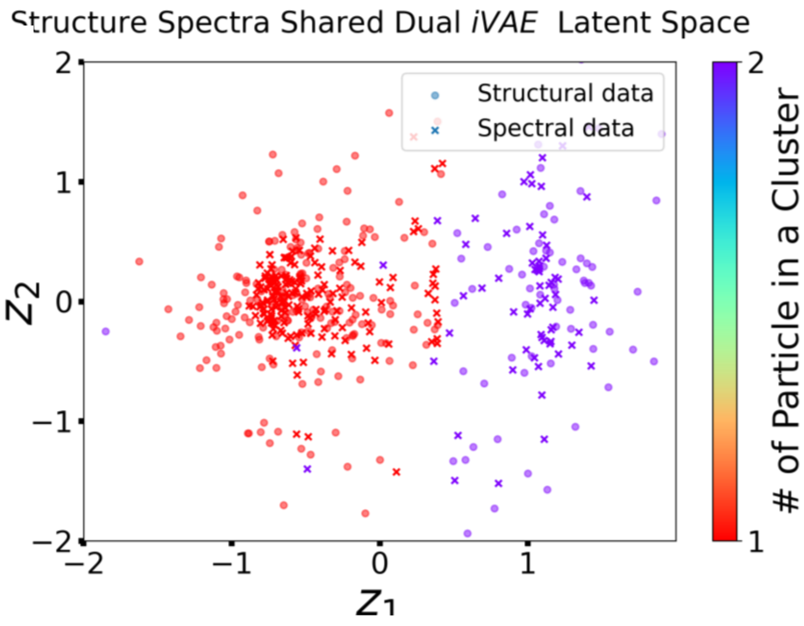
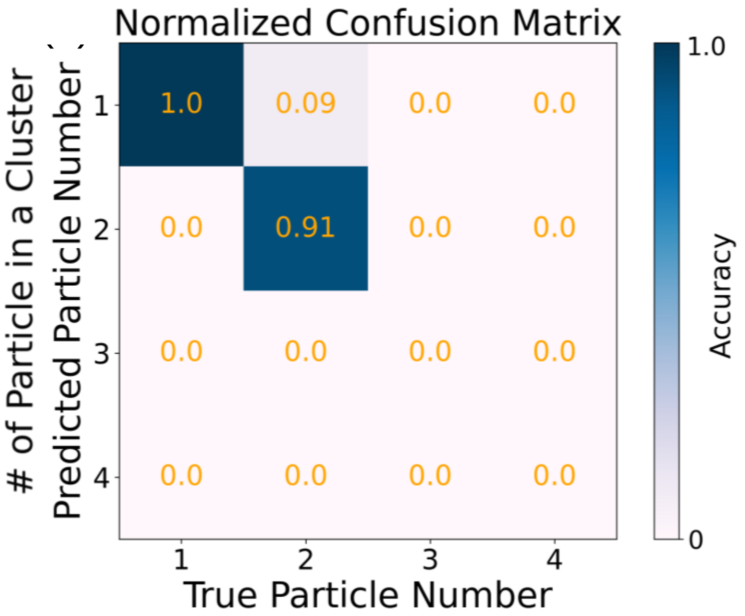
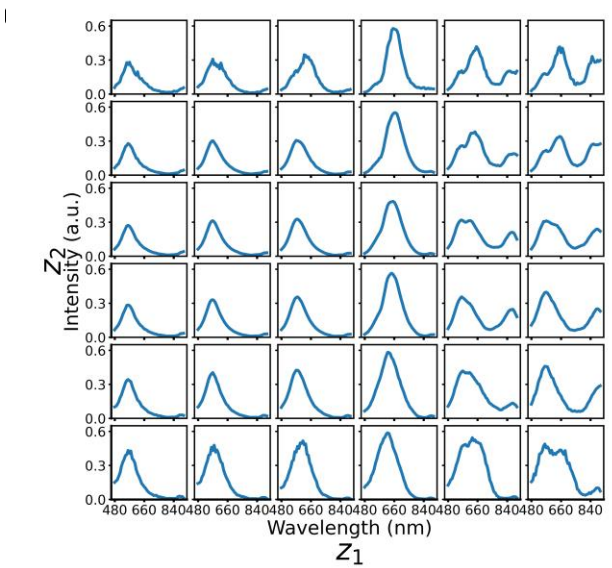
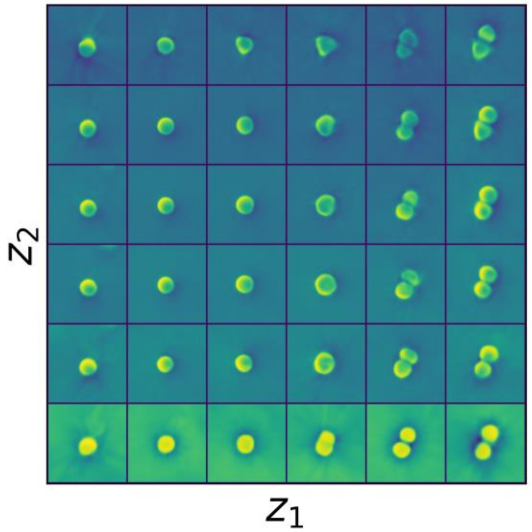
Dual VAE: Predictions for only 1 and 2 mers









Questions to ask when using ML

Data science:

- What is the dimensionality of feature and target spaces
- How variable are the features in these spaces (VAE can help)
- How much data do I have?

Domain knowledge:

- How predictive do I expect this relationship to be
- What other factors matter from materials side
- Can measurements introduce additional factors of variance?

Experiment planning:

- How much data can I have?
- Is it a static learning problem, or am I interested in ML-assisted experiment?