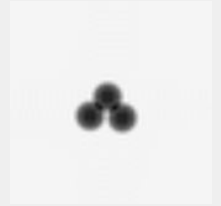# Exploring structural heterogeneity using X-ray single particle imaging and deep learning
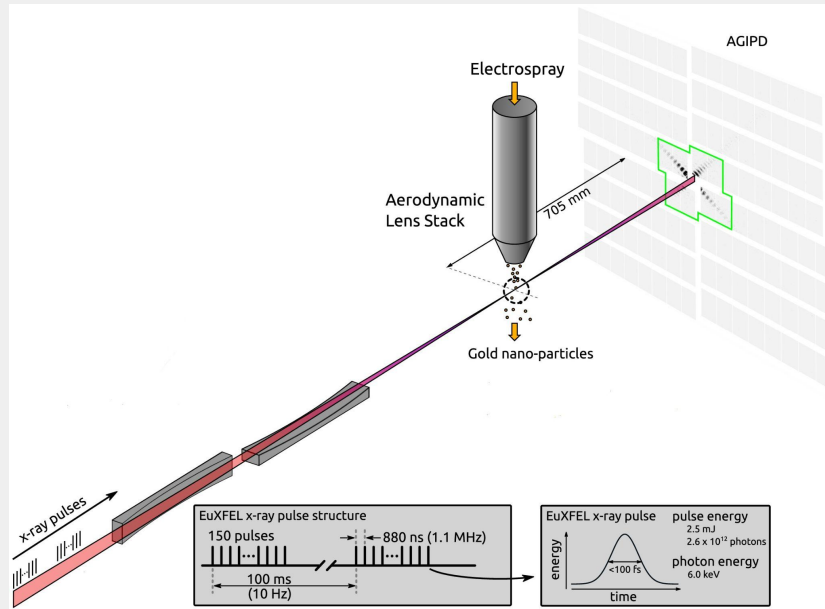
Round Table on DL

Abhishek Mall

Computational Nanoscale Imaging Group
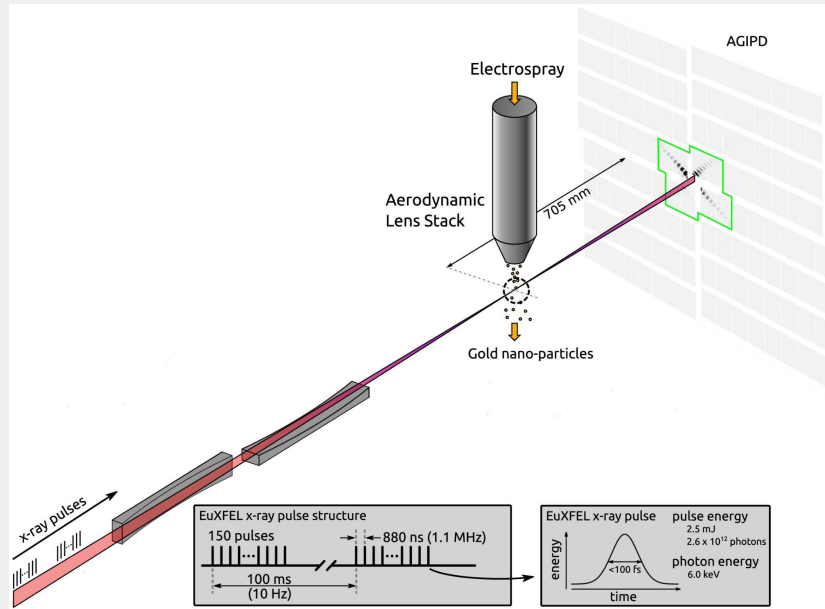
Max Planck Institute for the Structure and Dynamics of Matter

X-ray Single Particle Imaging(SPI)

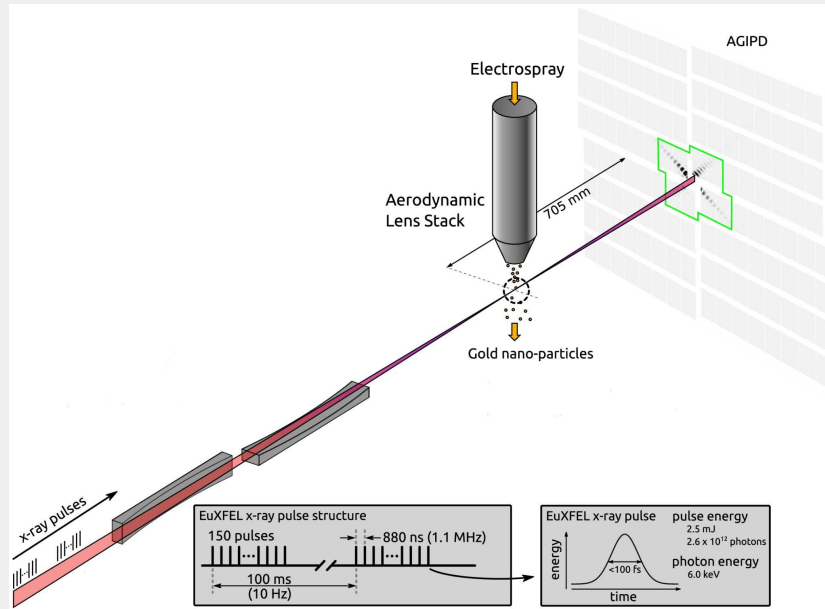- 3D diffractive imaging of nanoparticle ensembles using an x-ray laser," Optica 8, 15-23 (2021)

X-ray Single Particle Imaging(SPI)

- millions of diffraction patterns

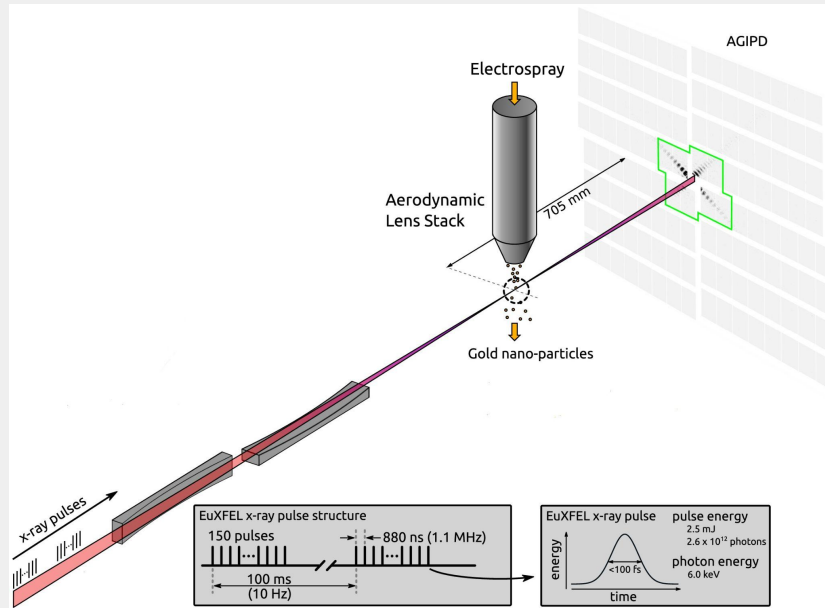- 3D diffractive imaging of nanoparticle ensembles using an x-ray laser," Optica 8, 15-23 (2021)

X-ray Single Particle Imaging(SPI)

- millions of diffraction patterns
- orientation determination

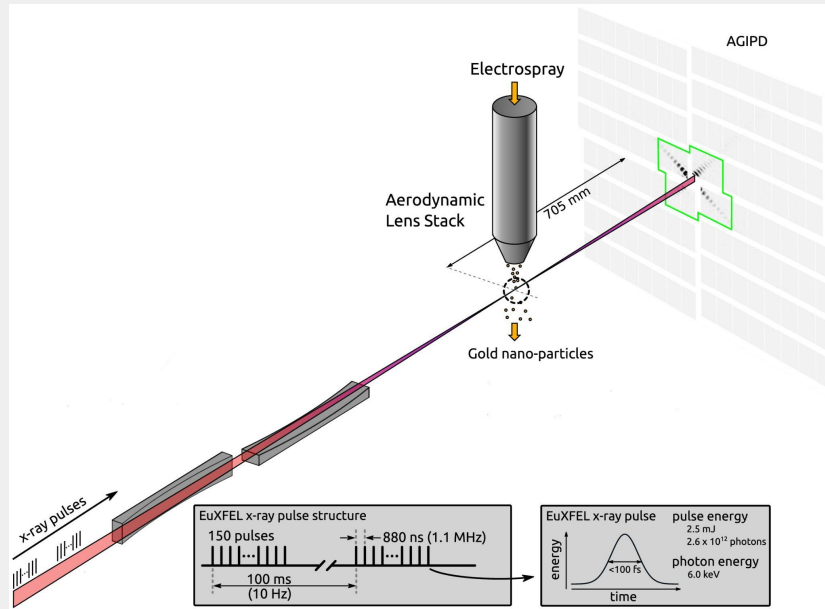- 3D diffractive imaging of nanoparticle ensembles using an x-ray laser," Optica 8, 15-23 (2021)

X-ray Single Particle Imaging(SPI)

- millions of diffraction patterns
- orientation determination
- reconstruction of 3D Structure

- 3D diffractive imaging of nanoparticle ensembles using an x-ray laser," Optica 8, 15-23 (2021)
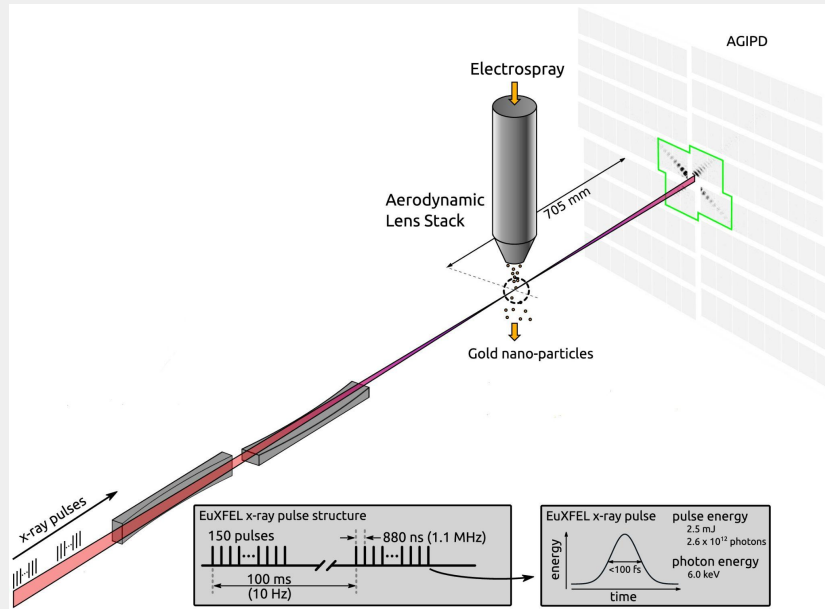
X-ray Single Particle Imaging(SPI)

- millions of diffraction patterns
- orientation determination
- reconstruction of 3D Structure
- shot-to-shot structural variation

- 3D diffractive imaging of nanoparticle ensembles using an x-ray laser," Optica 8, 15-23 (2021)
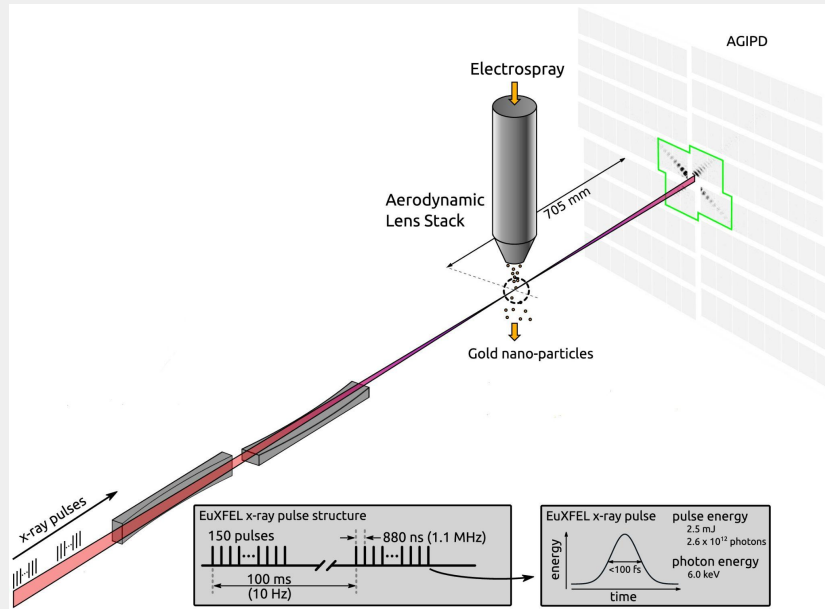
X-ray Single Particle Imaging(SPI)

- millions of diffraction patterns
- orientation determination
- reconstruction of 3D Structure
- shot-to-shot structural variation

- Studying two systems:
  a) Melting transition in Gold Nanoparticles

- 3D diffractive imaging of nanoparticle ensembles using an x-ray laser," Optica 8, 15-23 (2021)

X-ray Single Particle Imaging(SPI)

- millions of diffraction patterns
- orientation determination
- reconstruction of 3D Structure
- shot-to-shot structural variation

- Studying two systems:
  a) Melting transition in Gold Nanoparticles
  b) Structural changes in MS2 Virus

- 3D diffractive imaging of nanoparticle ensembles using an x-ray laser," Optica 8, 15-23 (2021)

Variational Autoencoder

- Zhuang, Yulong, et al. "Unsupervised learning approaches to characterizing heterogeneous samples using X-ray single-particle imaging." *IUCrJ* 9.2 (2022).
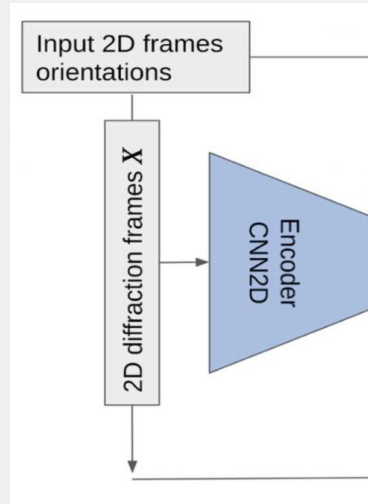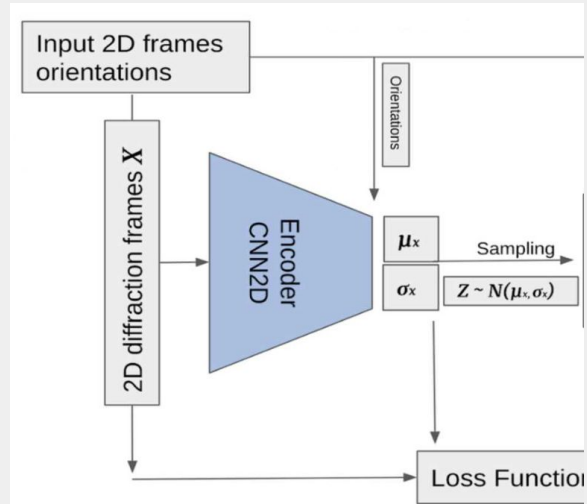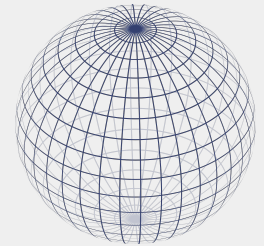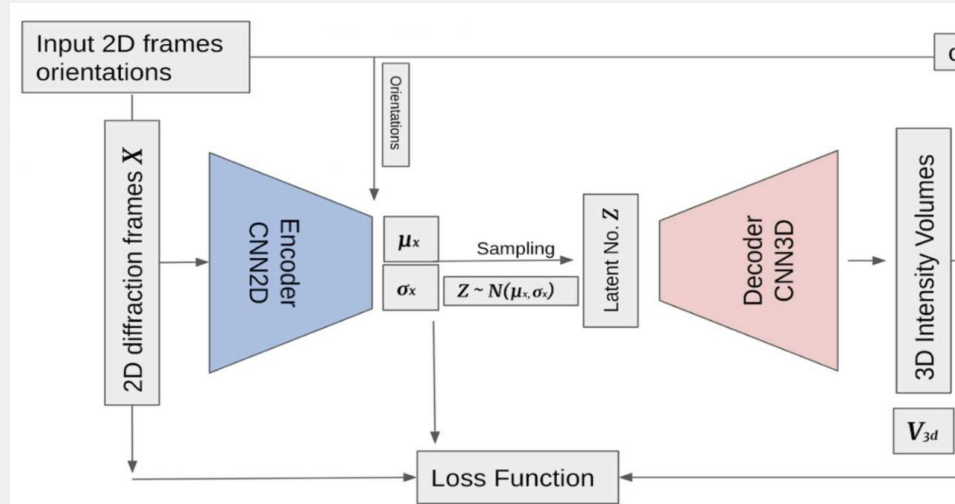
Variational Autoencoder
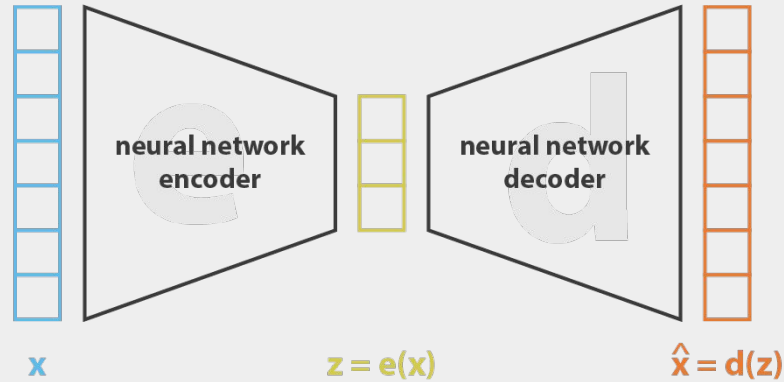
$$\text{loss} \; = \; || \, x - \hat{x} \, ||^2 \; = \; || \, x - d(z) \, ||^2 \; = \; || \, x - d(e(x)) \, ||^2$$

- Zhuang, Yulong, et al. "Unsupervised learning approaches to characterizing heterogeneous samples using X-ray single-particle imaging." *IUCrJ* 9.2 (2022).
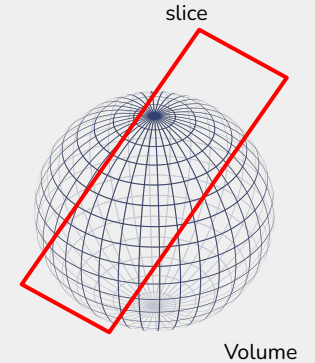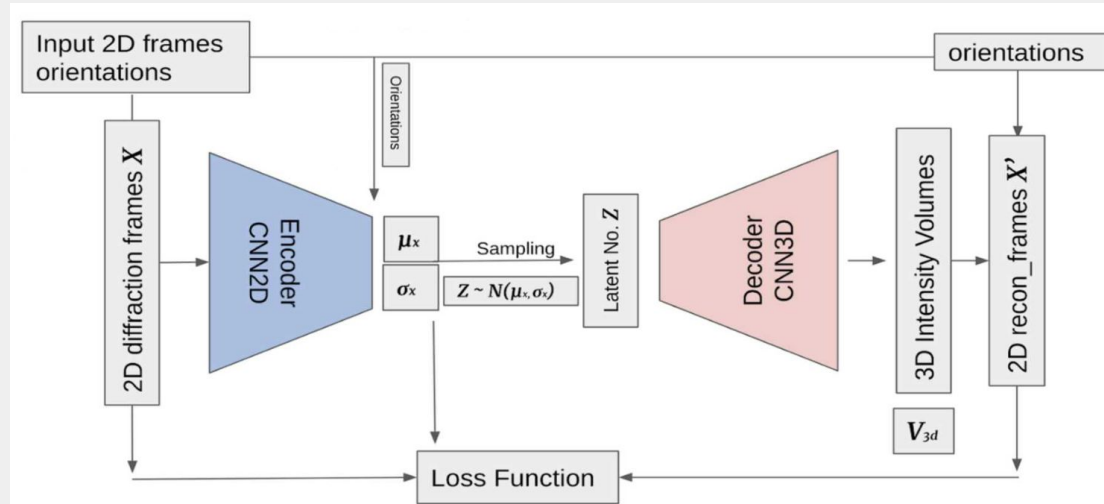
Variational Autoencoder
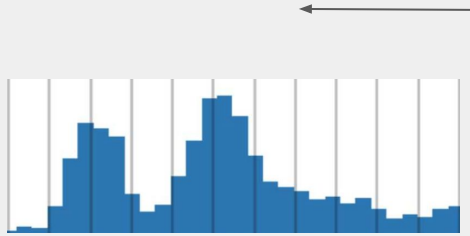
- Zhuang, Yulong, et al. "Unsupervised learning approaches to characterizing heterogeneous samples using X-ray single-particle imaging." *IUCrJ* 9.2 (2022).

Variational Autoencoder

- Zhuang, Yulong, et al. "Unsupervised learning approaches to characterizing heterogeneous samples using X-ray single-particle imaging." *IUCrJ* 9.2 (2022).

Variational Autoencoder

Volume

- Zhuang, Yulong, et al. "Unsupervised learning approaches to characterizing heterogeneous samples using X-ray single-particle imaging." *IUCrJ* 9.2 (2022).
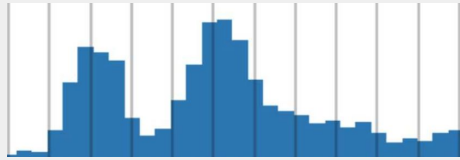
Variational Autoencoder

- Zhuang, Yulong, et al. "Unsupervised learning approaches to characterizing heterogeneous samples using X-ray single-particle imaging." *IUCrJ* 9.2 (2022).
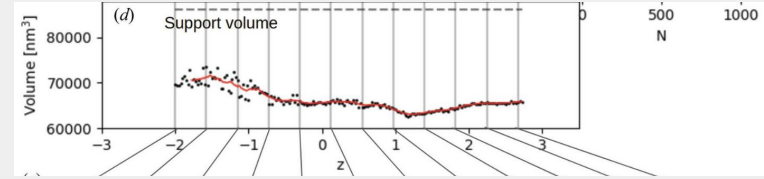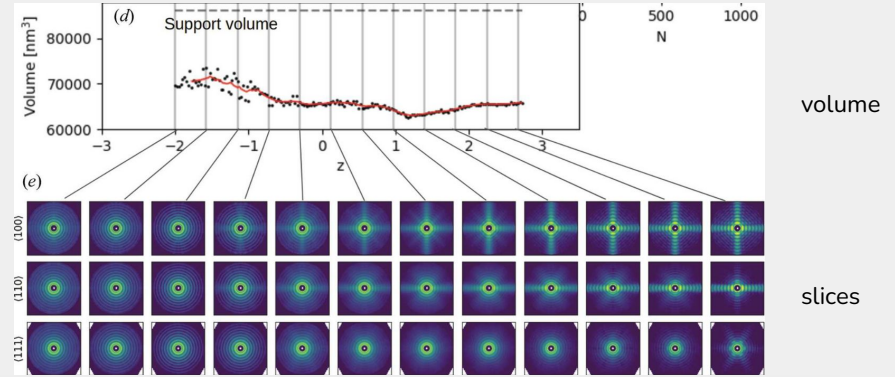
Melting Transition in AuNP

Histogram of z

- Zhuang, Yulong, et al. "Unsupervised learning approaches to characterizing heterogeneous samples using X-ray single-particle imaging." *IUCrJ* 9.2 (2022).
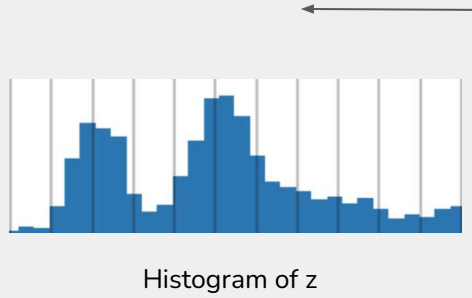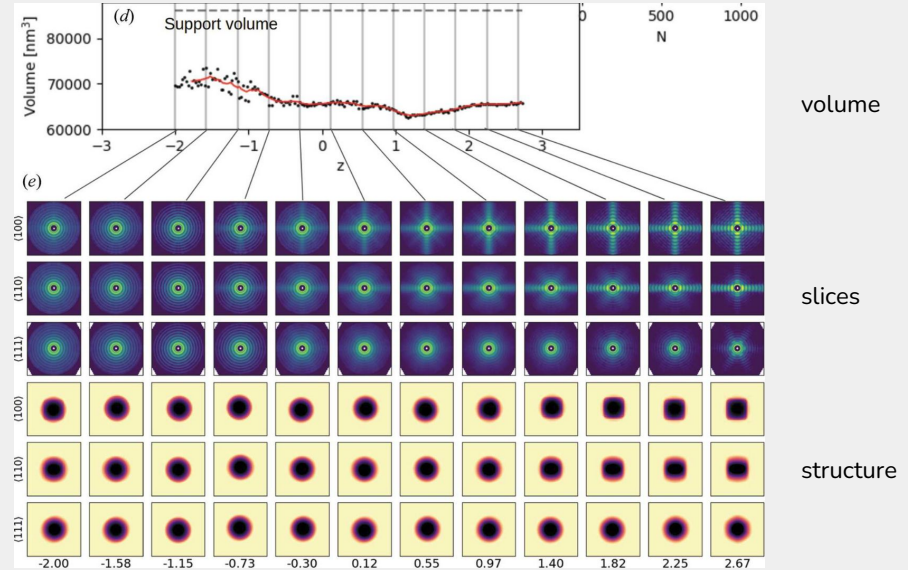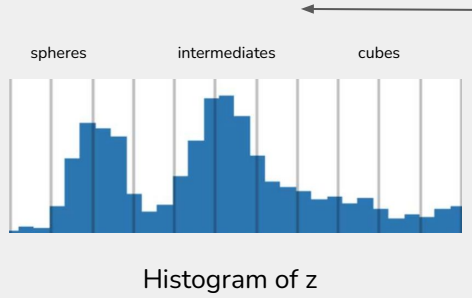
Melting Transition in AuNP
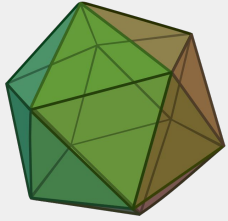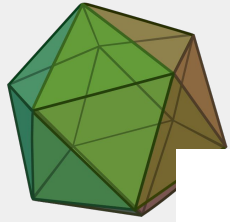

Histogram of z

volume

- Zhuang, Yulong, et al. "Unsupervised learning approaches to characterizing heterogeneous samples using X-ray single-particle imaging." *IUCrJ* 9.2 (2022).

Melting Transition in AuNP

Histogram of z

volume

slices

● Zhuang, Yulong, et al. "Unsupervised learning approaches to characterizing heterogeneous samples using X-ray single-particle imaging." *IUCrJ* 9.2 (2022).

Melting Transition in AuNP

Histogram of z

- Zhuang, Yulong, et al. "Unsupervised learning approaches to characterizing heterogeneous samples using X-ray single-particle imaging." *IUCrJ* 9.2 (2022).

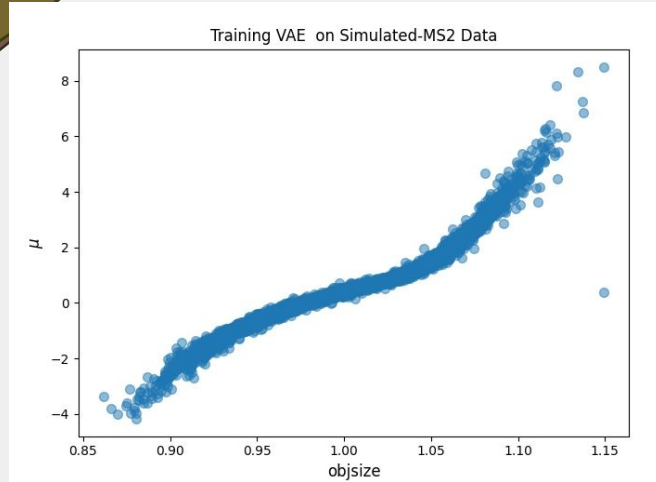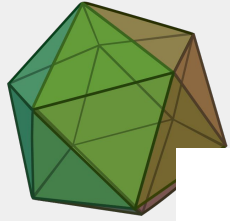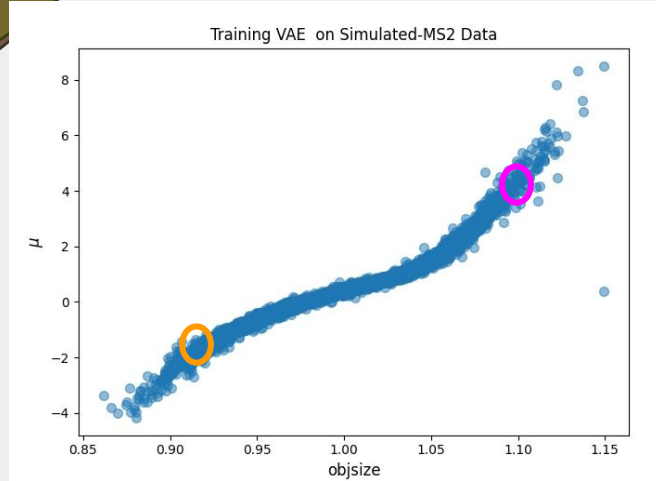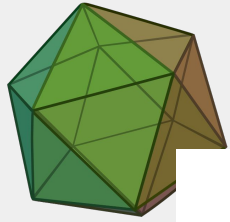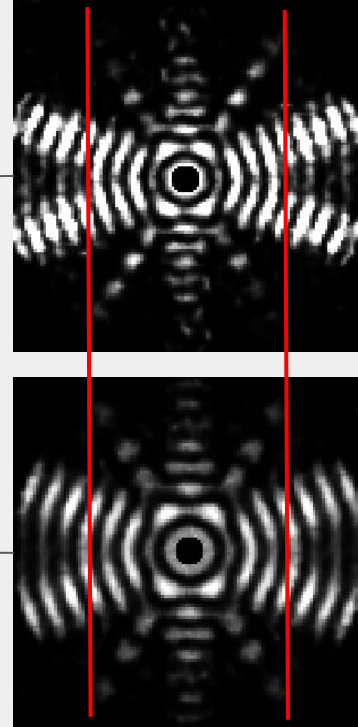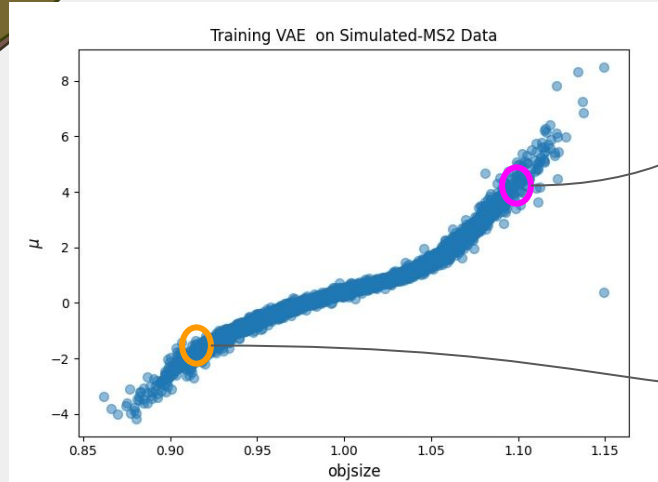# Structural Landscape of MS2 Bacteriophage(ongoing)

size variation

Structural Landscape of MS2 Bacteriophage(ongoing)

size variation

Training VAE on Simulated-MS2 Data

Structural Landscape of MS2 Bacteriophage(ongoing)

size variation

Training VAE on Simulated-MS2 Data

Structural Landscape of MS2 Bacteriophage(ongoing)
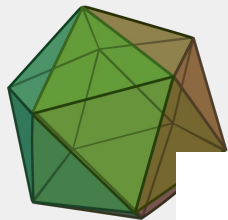
size variation

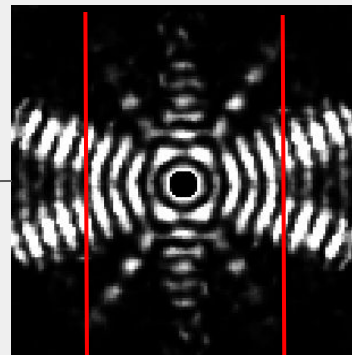Training VAE on Simulated-MS2 Data

Slicing through reconstructed volume

Structural Landscape of MS2 Bacteriophage(ongoing)
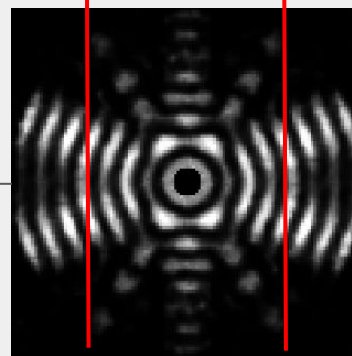

size variation

Training VAE on Simulated-MS2 Data
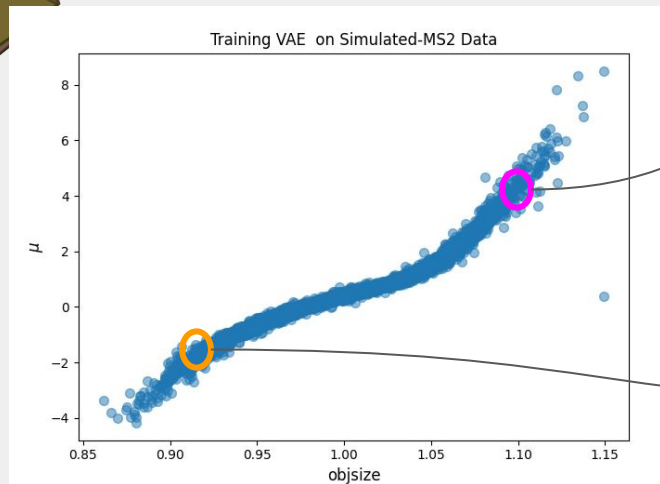
Larger Particle

Slicing through reconstructed volume

Smaller Particle
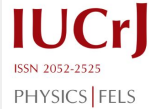
Summary

1. **Unsupervised learning approaches to characterizing heterogeneous samples using X-ray single-particle imaging**

   IUCrJ
   ISSN 2052-2525
   PHYSICS | FELS

2. Uncovering Structural Landscape of MS2 Bacteriophage via Deep Learning

Collaborators: EuXFEl, CFEL, UHH, NUS

Anna Munke, Michael Rütten, Tobias Beck, Anton Barty, Richard Bean, Johan Bielecki, Martin Bergemann, Benedikt J. Daurer, Tomas Ekeberg, Armando D. Estillore, Hans Fangohr, Klaus Giewekemeyer, Mark S. Hunter, Mikhail Karnevskiy, Richard A. Kirian, Henry Kirkwood, Yoonhee Kim, Jayanath Koliyadu, Holger Lange, Romain Letrun, Jannik Lu¨bke, Thomas Michelat, Andrew J. Morgan, Nils Roth, Amit K. Samanta, Tokushi Sato, Marcin Sikorski, Florian Schulz, John C. H. Spence, Patrik Vagovic, Tamme Wollweber, Lena Worbs, P. Lourdu Xavier, Oleksandr Yefanov, Filipe R. N. C. Maia, Daniel A. Horke, Jochen Ku¨pper, N. Duane Loh, Adrian P. Mancuso, Henry N. Chapman

Acknowledgements

1.
Unsupervised learning approaches to characterizing heterogeneous samples using X-ray single-particle imaging

2. Uncovering Structural Landscape of MS2 Bacteriophage via Deep Learning

Yulong Zhuang

Shen Zhou

Collaborators: EuXFEl, CFEL, UHH, NUS

Acknowledgements

Thank You. Questions!