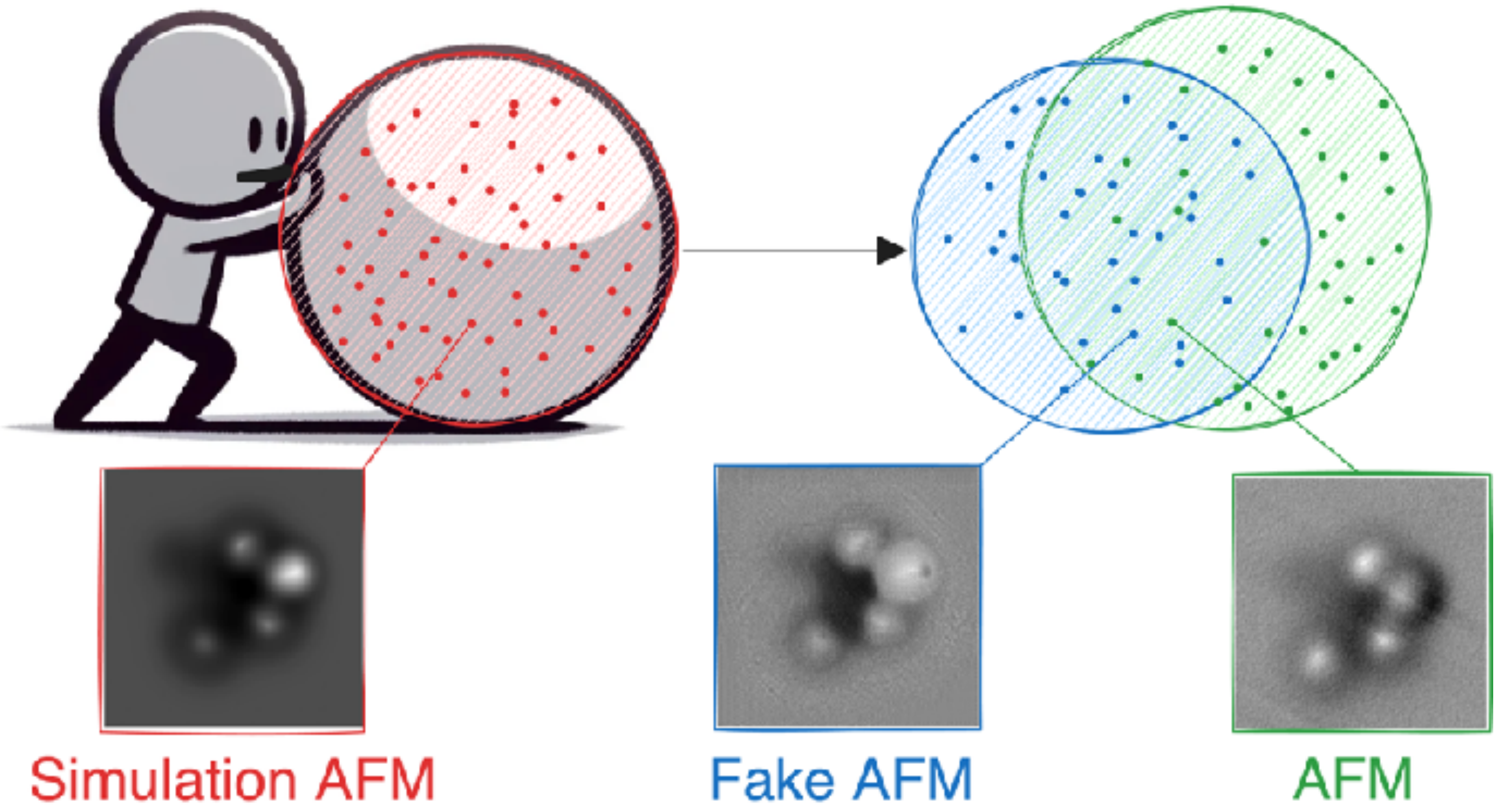
Enhancing Atomic Force Microscopy Image Analysis: Style Translation and Data Augmentation

Jie Huang (jie.huang@aalto.fi)

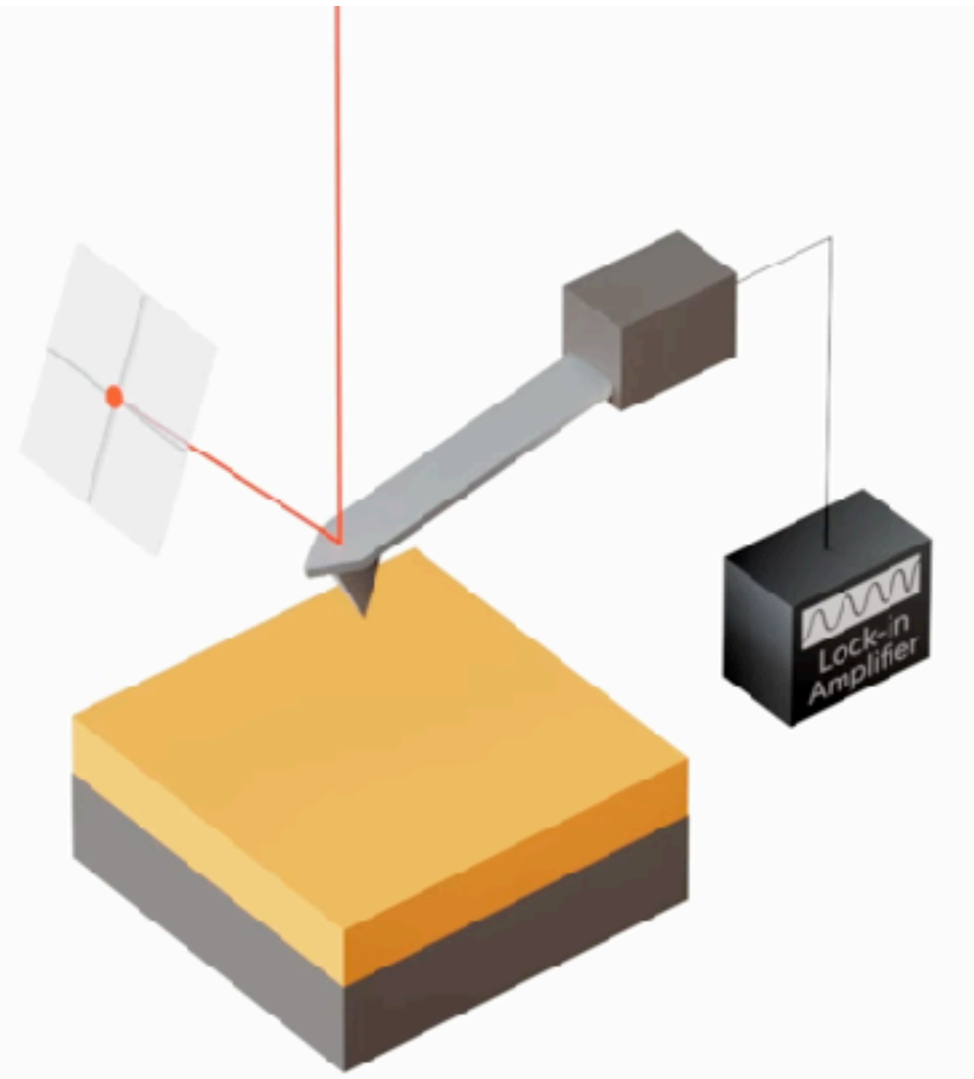
17/09/2024
MLM24, Kanazawa, Japan

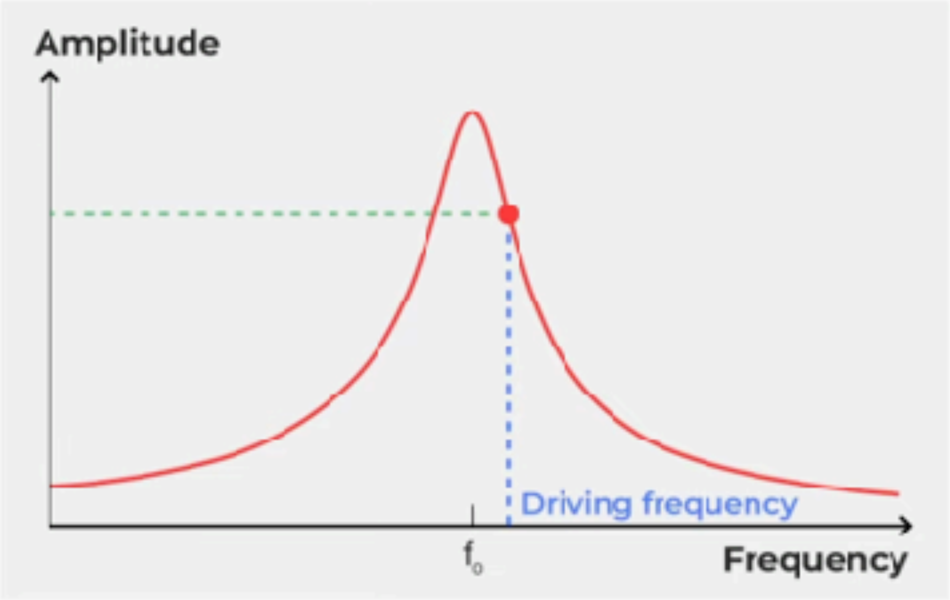


Surfaces and Interfaces at the Nanoscale (SIN)
Aalto University School of Science

Background

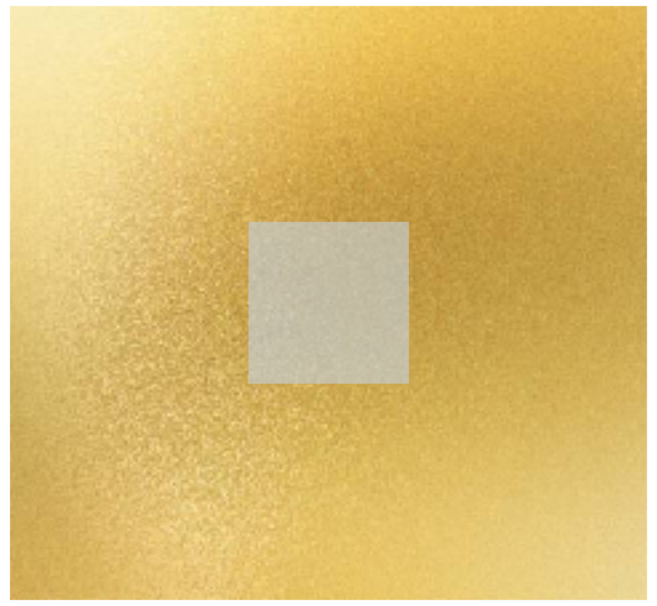
Atomic force microscopy (AFM)





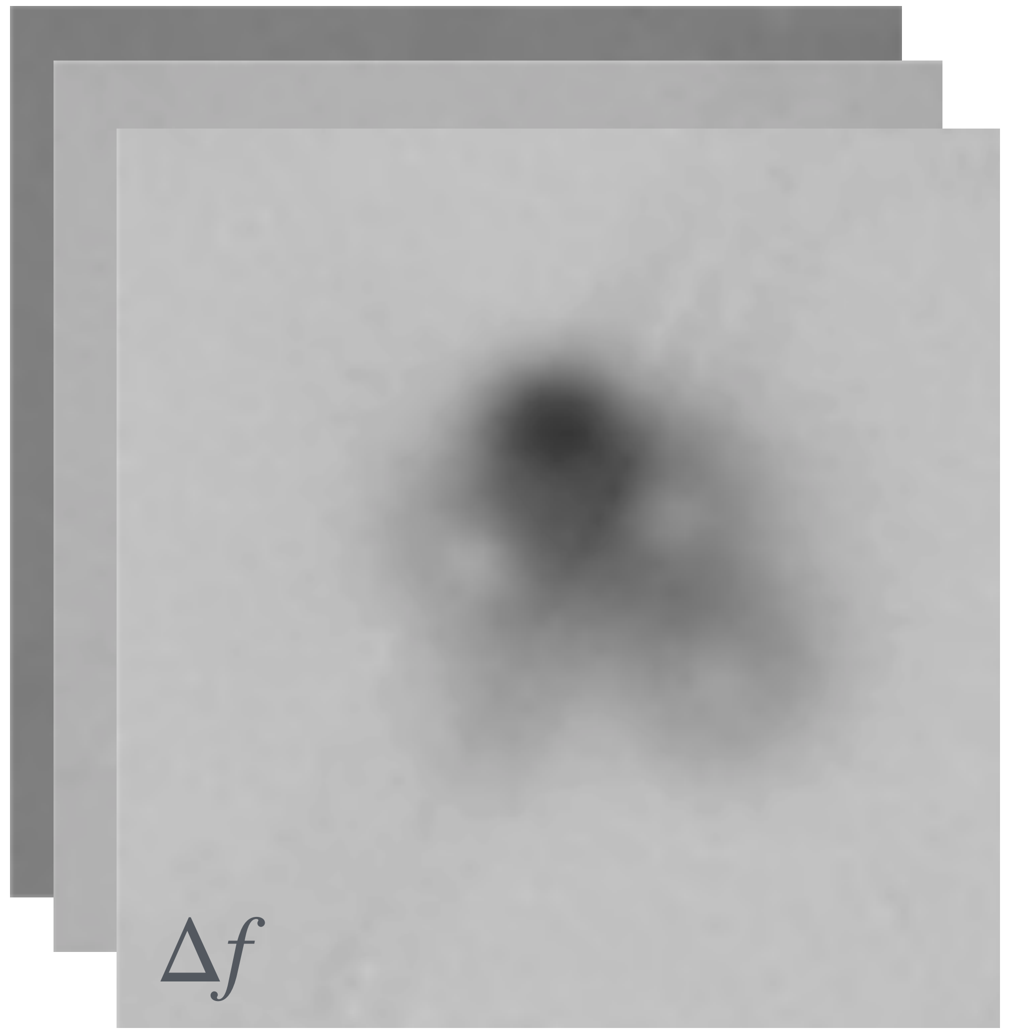
$$\Delta f = f - f_0$$

Prepare substrate and sample in lab



AFM →

AFM images.



Can we know the exact configuration/structure?

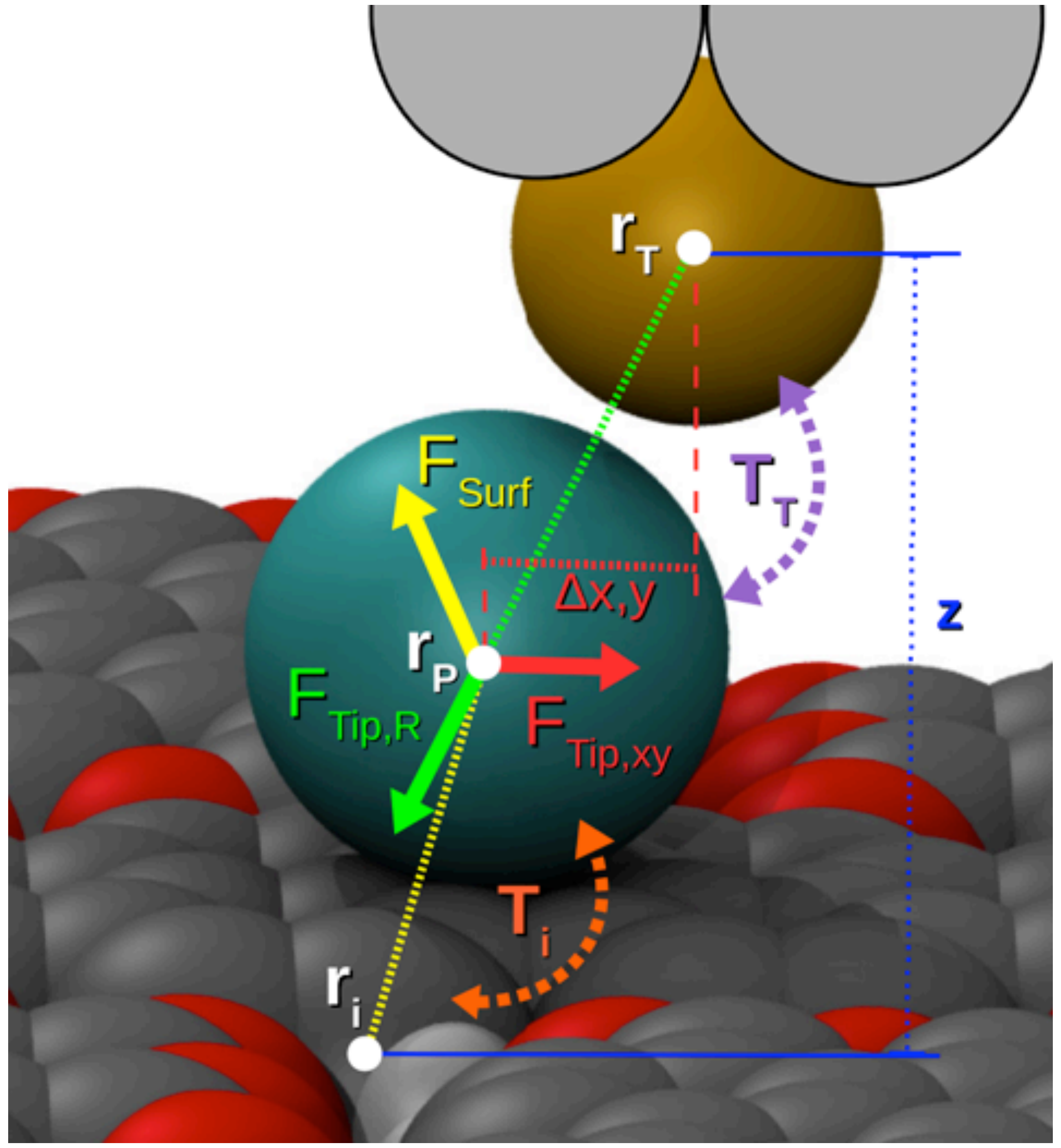
Where is O and H if it's a sample of water molecules?

Non-contact mode

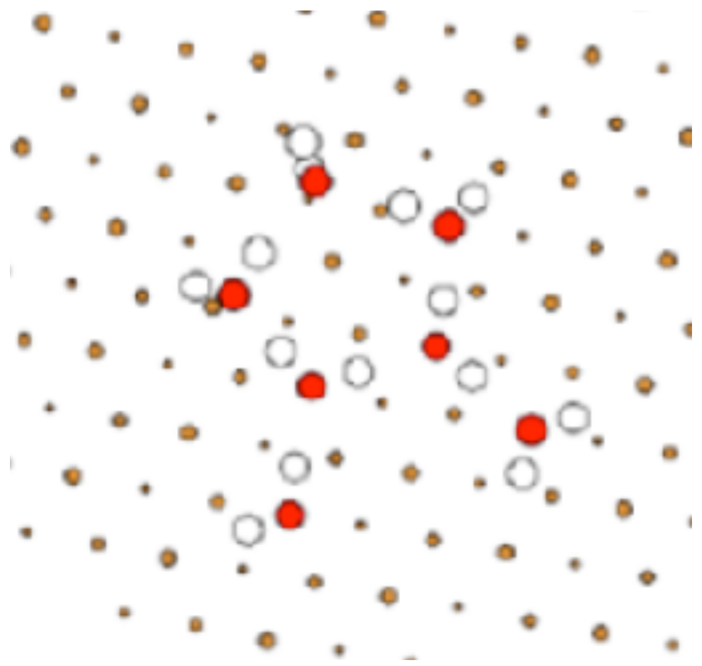
https://youtu.be/K9FgPWK3Co4?si=hnL9WH7ONWRUkVxJ

Background

Probe-Particle AFM (PPAFM)

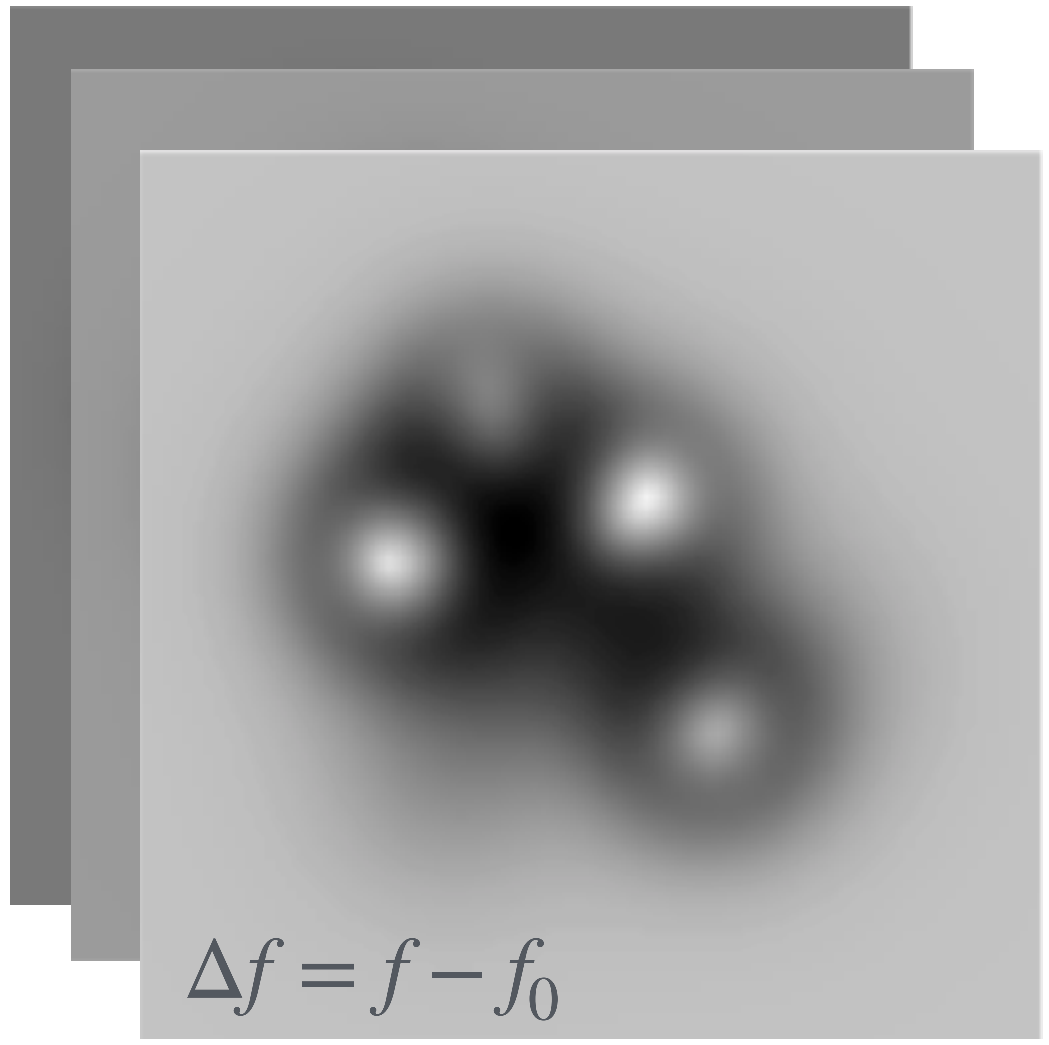


Prepare substrate and sample using DFT calculations



PPAFM →

Simulation AFM images.



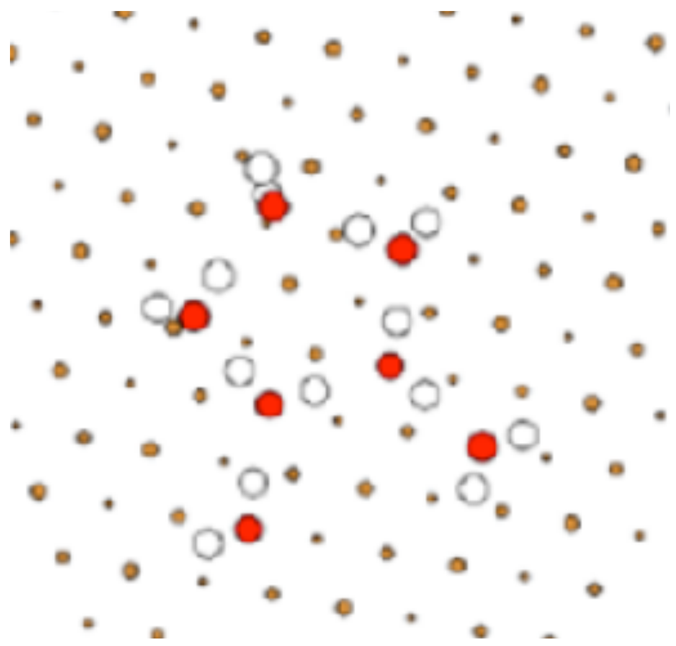
Where is O and H?

https://github.com/Probe-Particle/ppafm

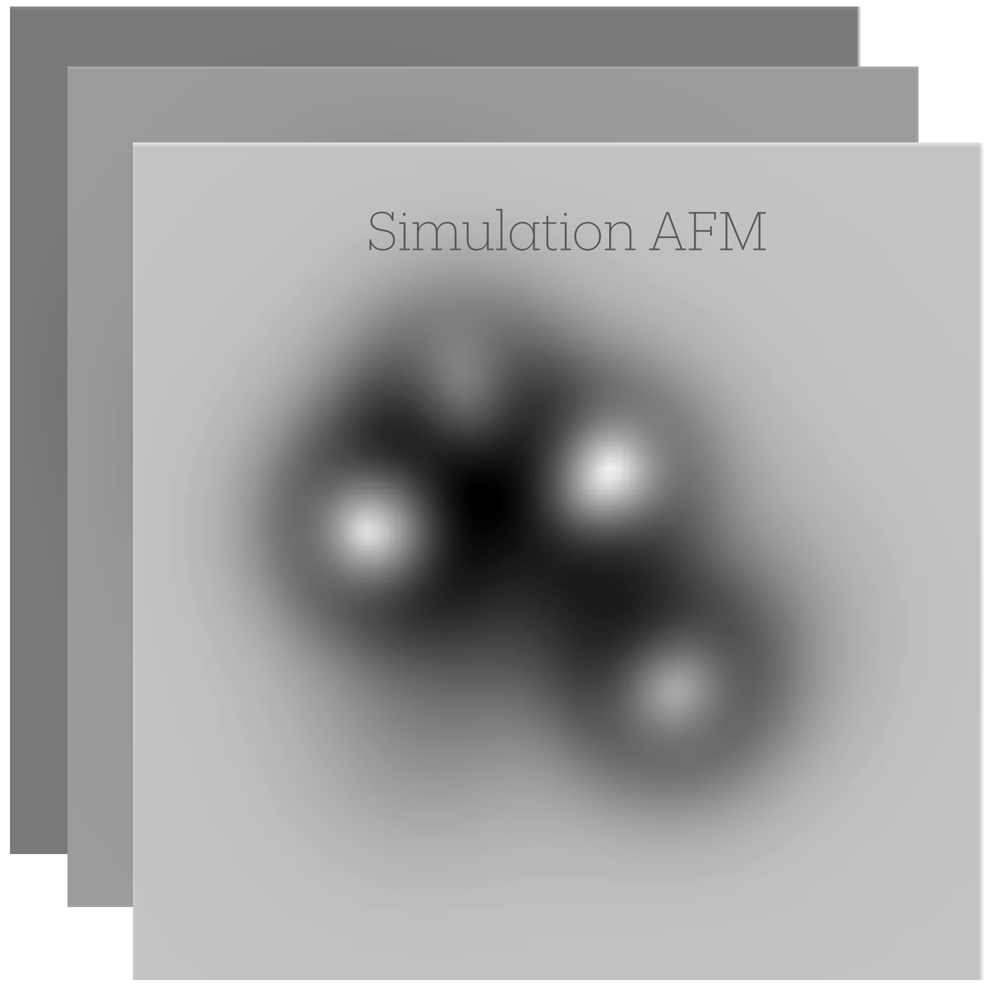
Hapala et al., Phys. Rev. Lett., 113, 226101 (2014).

Priante et al., ACS Nano, 2024, DOI: 10.1021/acsnano.3c10958.

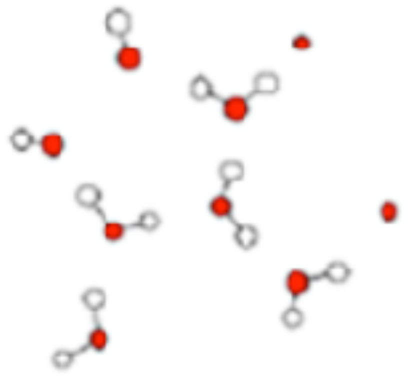
Machine Learning (ML) Applications

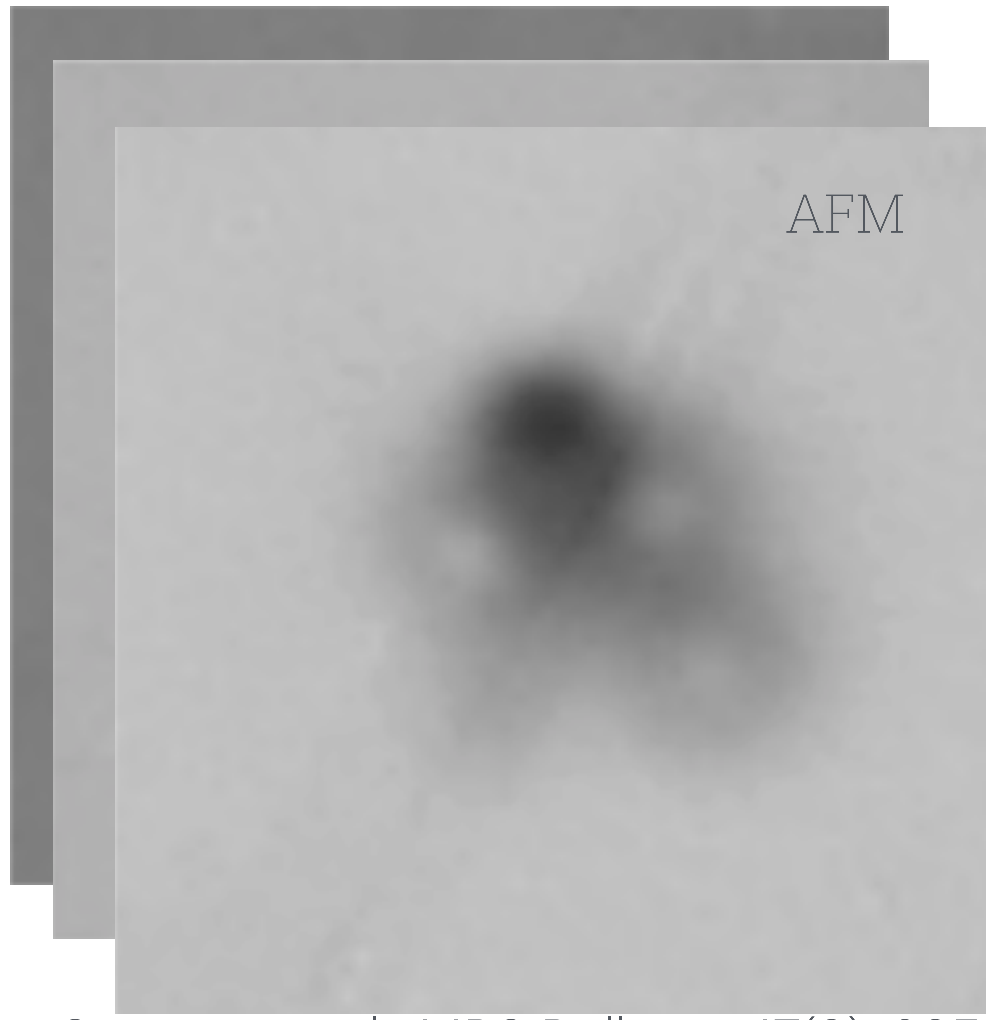


PPAFM

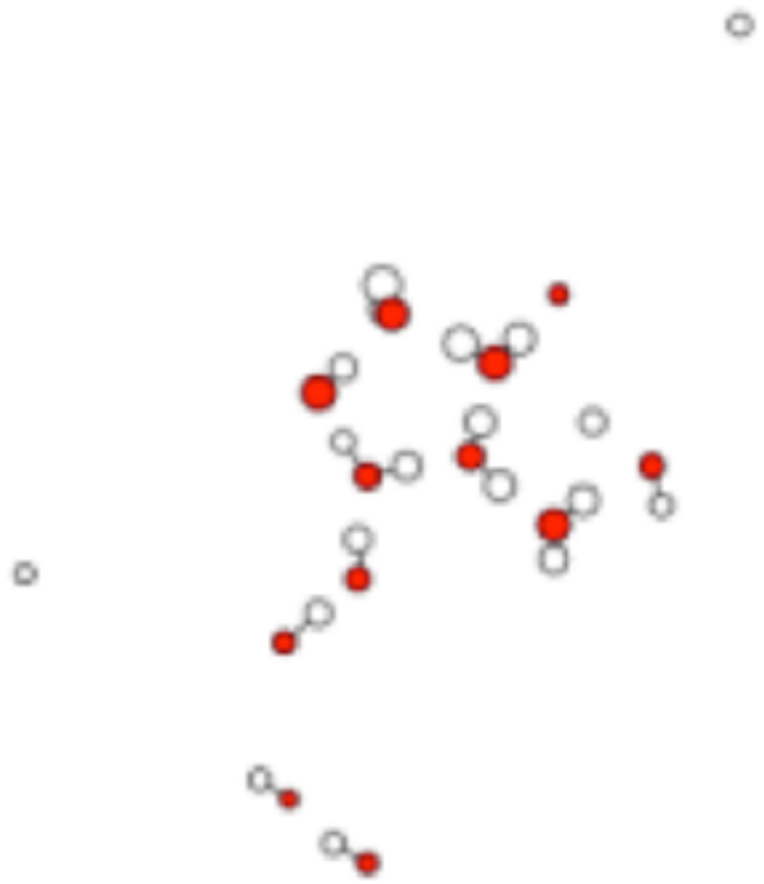


ML model





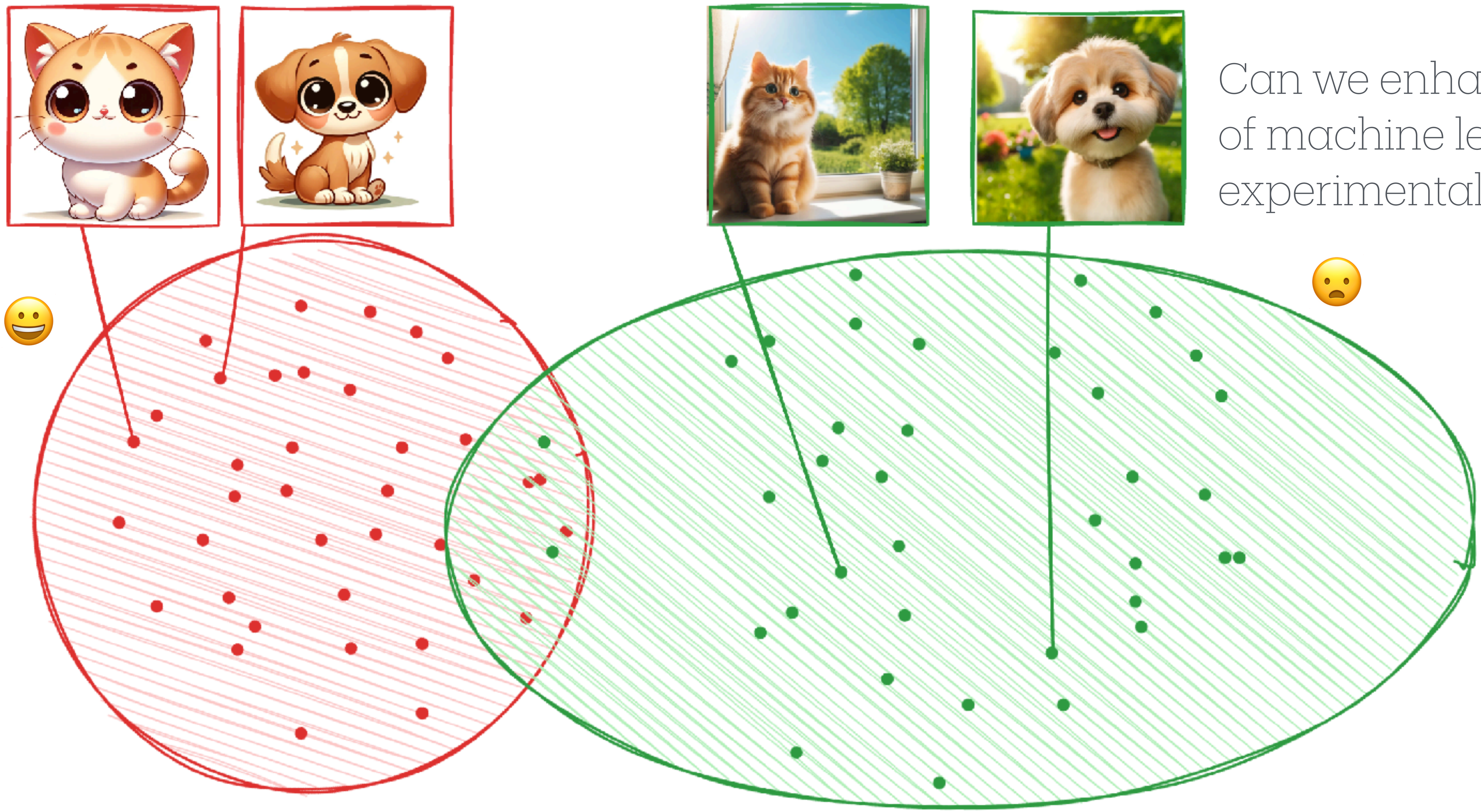
ML model



What happened here?

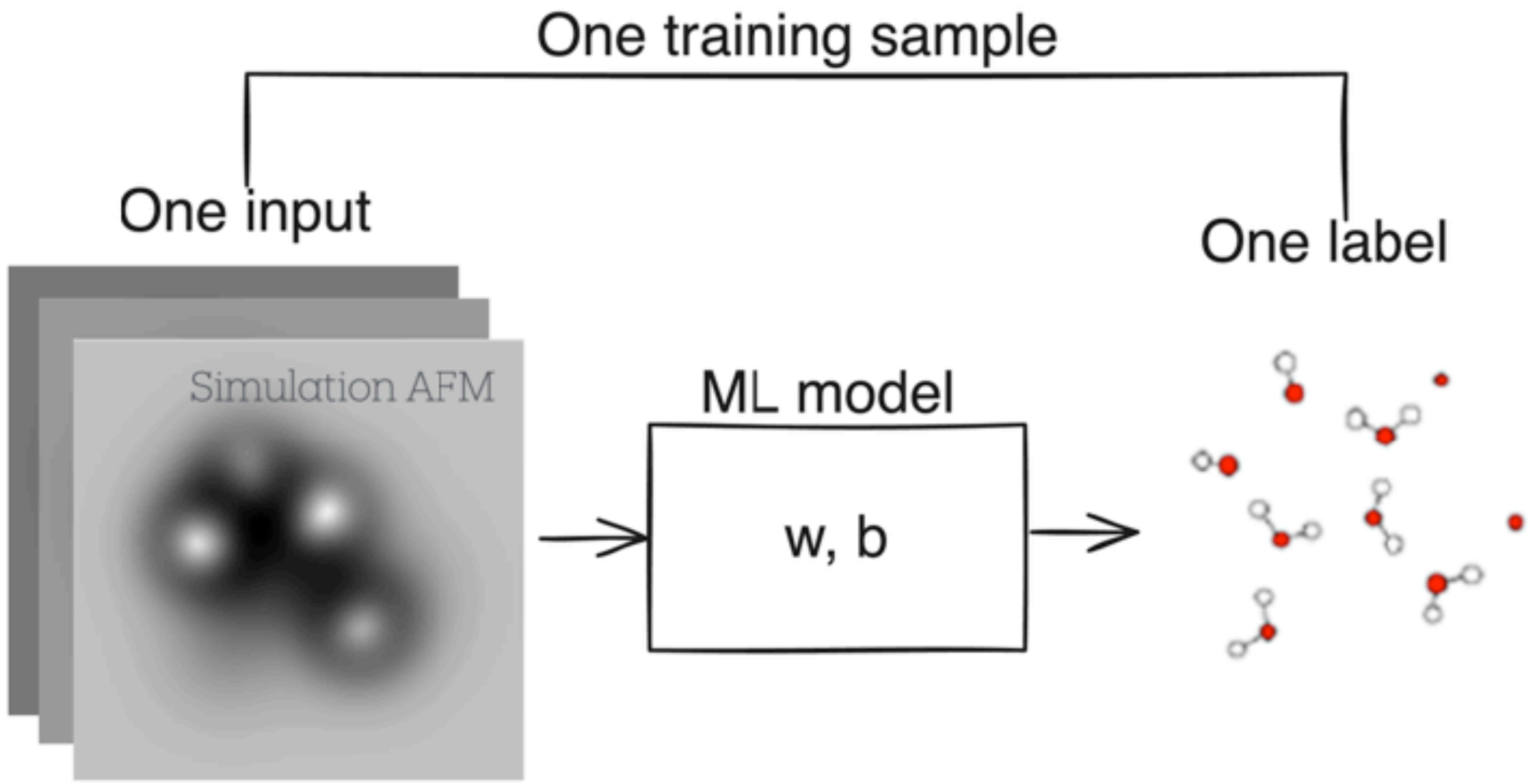
Oinonen et al., MRS Bulletin, 47(9), 895-905 (2022), DOI: 10.1557/s43577-022-00324-3.
Oinonen et al., ACS Nano, 16(1), 89-97 (2021), DOI: 10.1021/acsnano.1c06840.
Kurki et al., *ACS Nano*, 18(17), 11130-11138 (2024), DOI: 10.1021/acsnano.3c12654.
Priante et al., ACS Nano, (2024), DOI: 10.1021/acsnano.3c10958.

Distribution shift



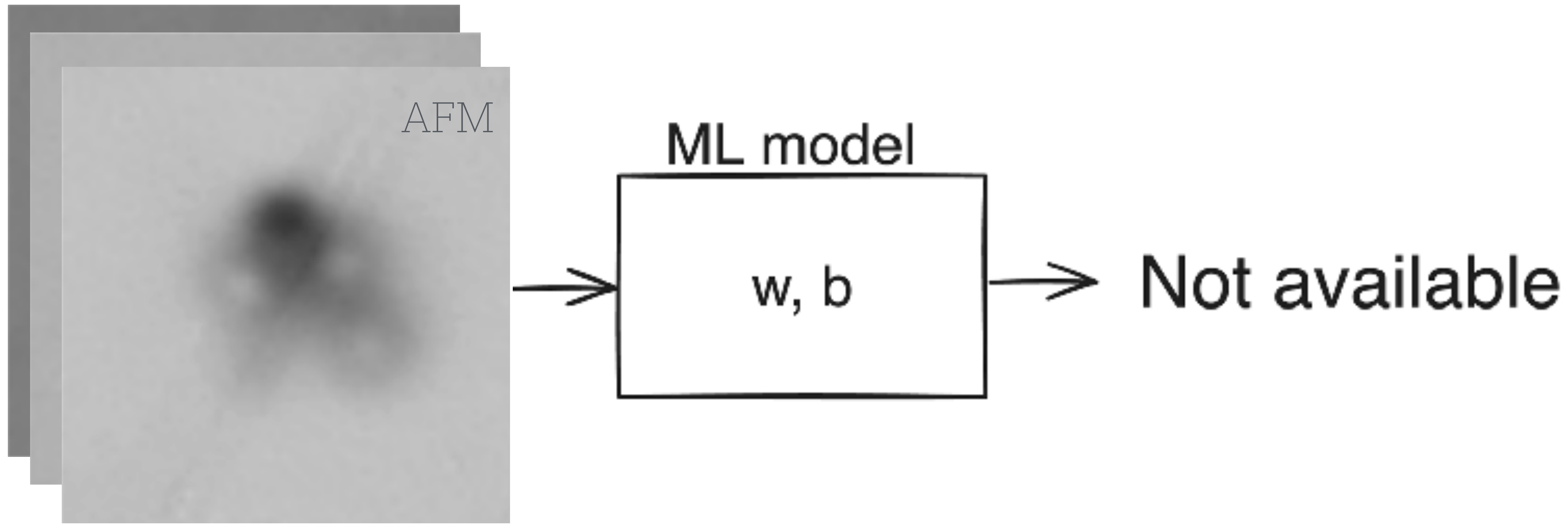
Can we enhance the performance of machine learning(ML) models on experimental AFM images?

Challenges in machine learning



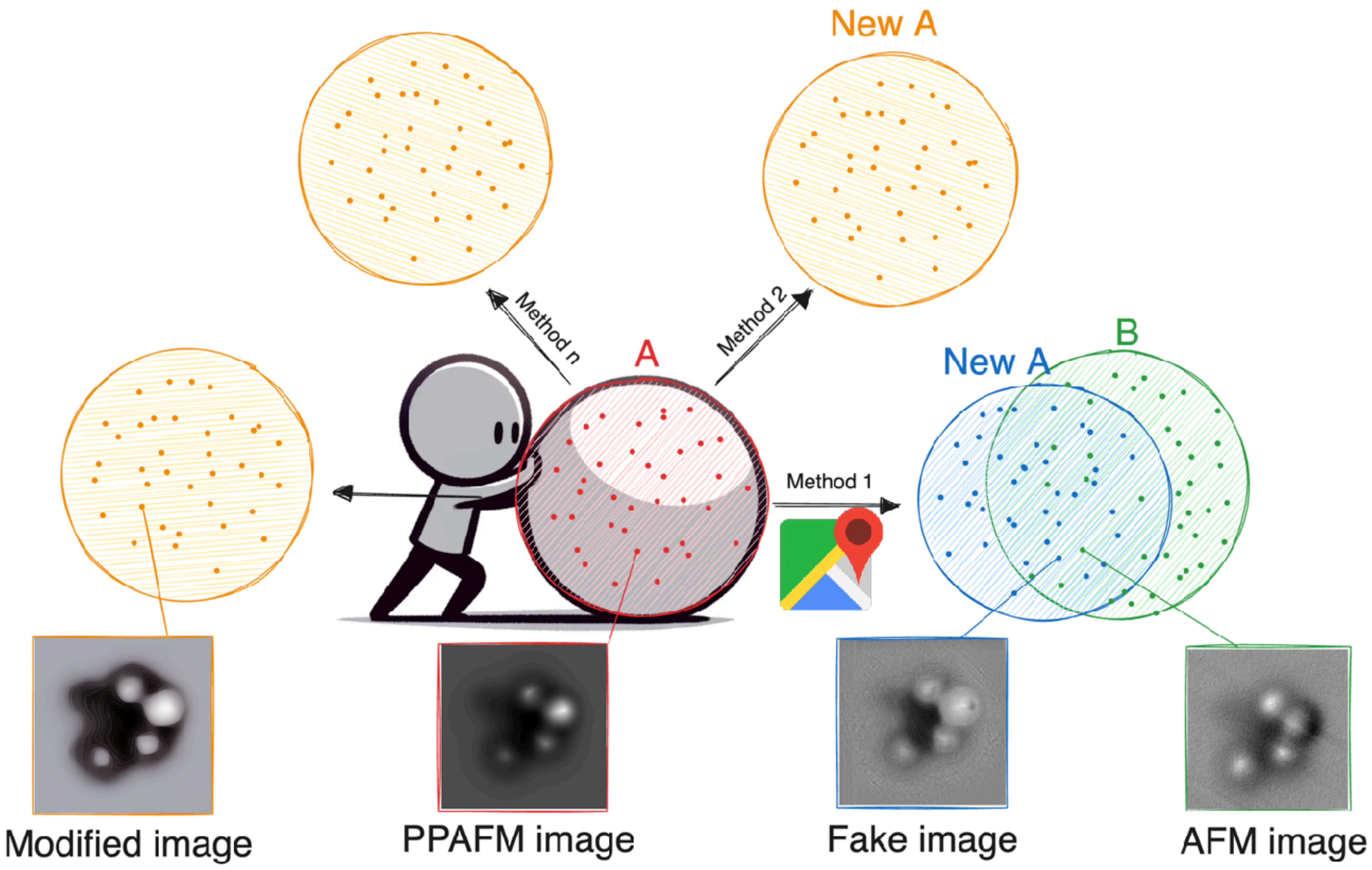
16 000 training samples
in Water-Au111 dataset.

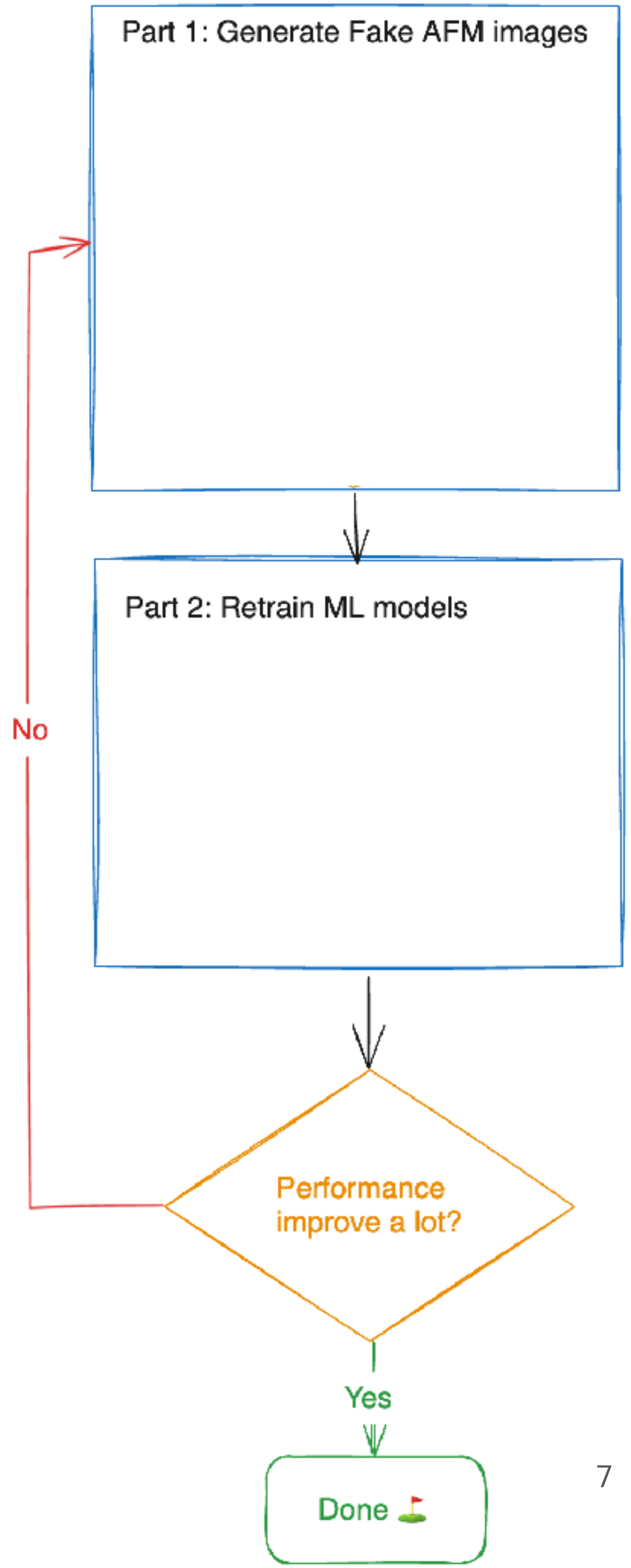
Cost too much money & time.



Label not available.

Hypothesis & Workflow

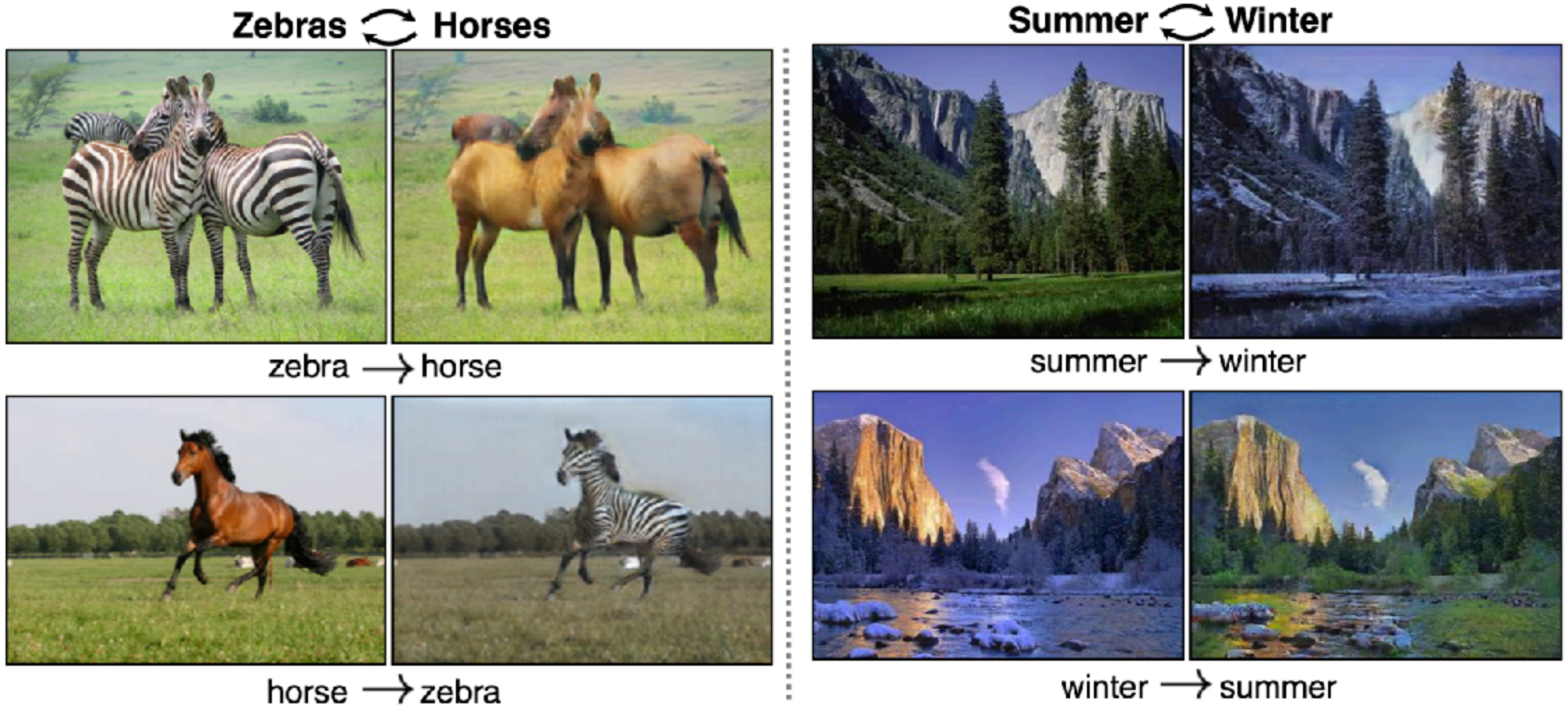


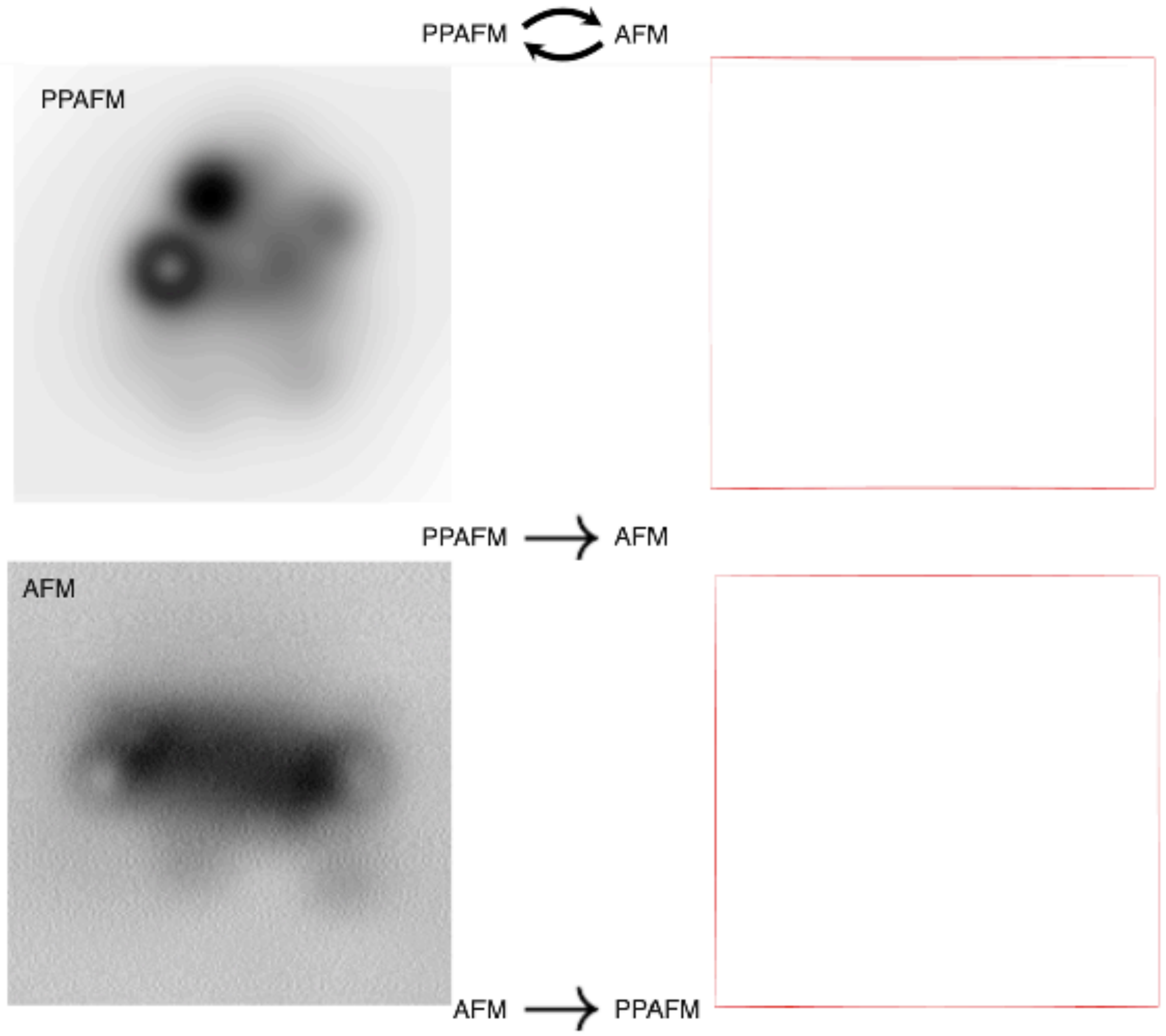


https://myedit.online/en/photo-editor/image-cartoonizer

How to generate fake AFM?

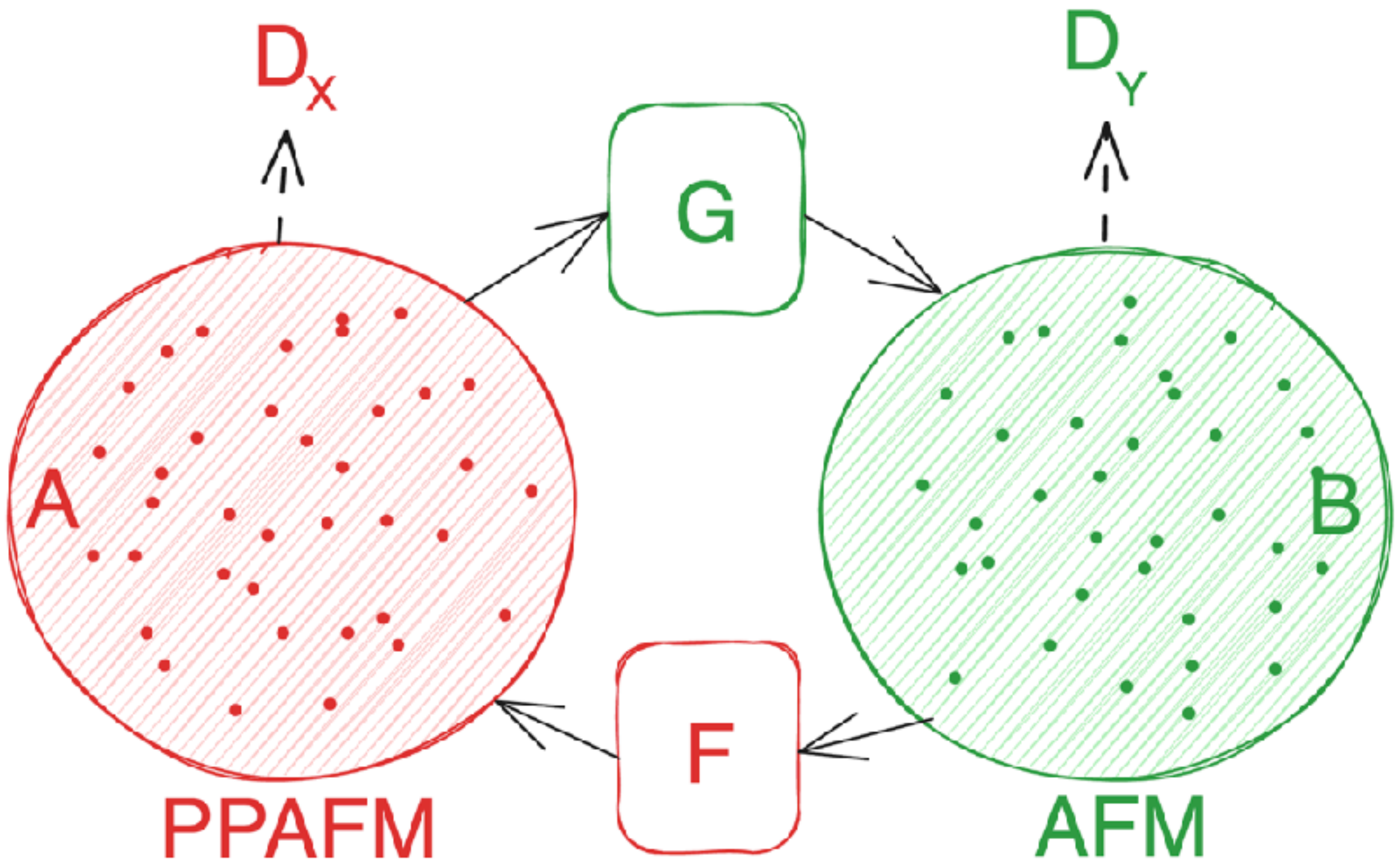
CycleGAN





Zhu et al., *arXiv:1703.10593* (2017).

Style translation between PPAFM & AFM

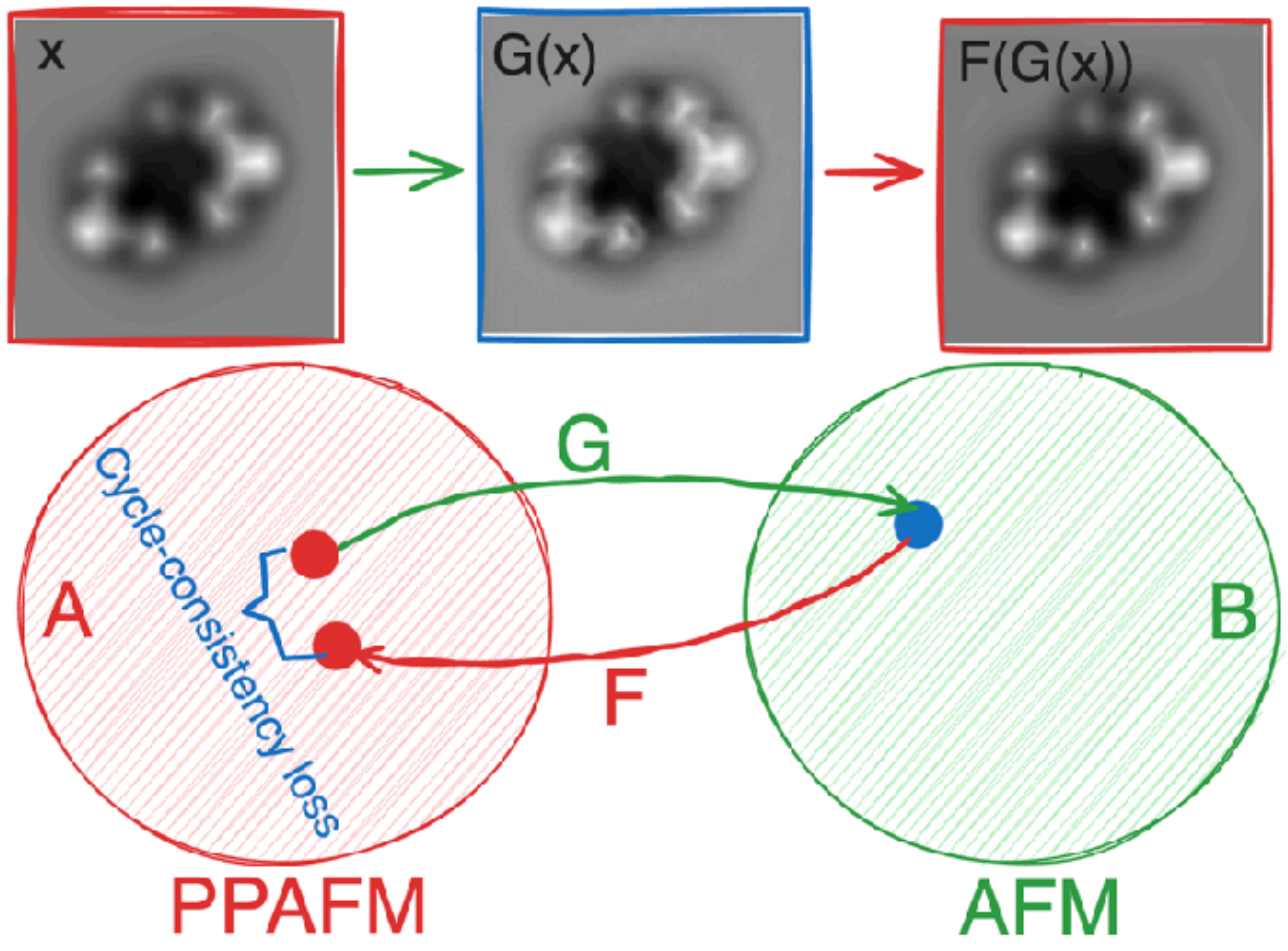


$$\mathcal{L}_{\mathrm{GAN}}(G, D_Y, X, Y) = \mathbb{E}_{y \sim p_{\mathrm{data}}(y)}[\log D_Y(y)] + \mathbb{E}_{x \sim p_{\mathrm{data}}(x)}[\log(1 - D_Y(G(x))]$$

$$G^* = \arg\min_G \mathcal{L}_{\mathrm{GAN}}(G, D_Y, X, Y)$$

$$D_Y^* = \arg\max_D \mathcal{L}_{\mathrm{GAN}}(G, D_Y, X, Y)$$

$$G^*, D_Y^* = \arg\min_G \max_D \mathcal{L}_{\mathrm{GAN}}(G, D_Y, X, Y)$$

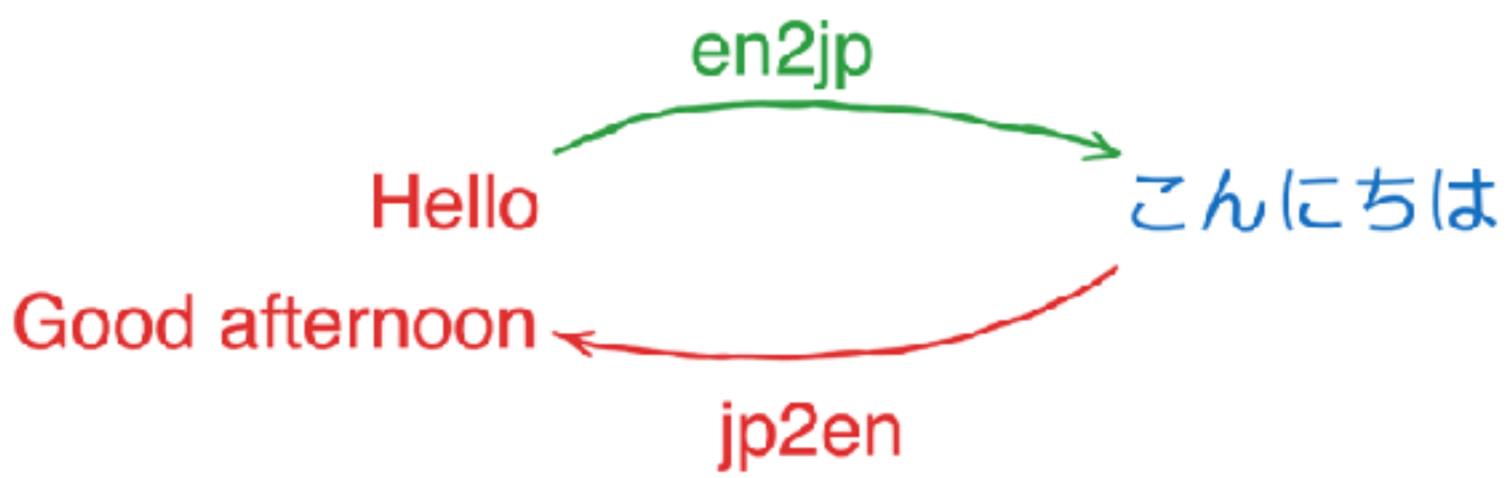


$$x \rightarrow G(x) \rightarrow F(G(x)) \approx x$$

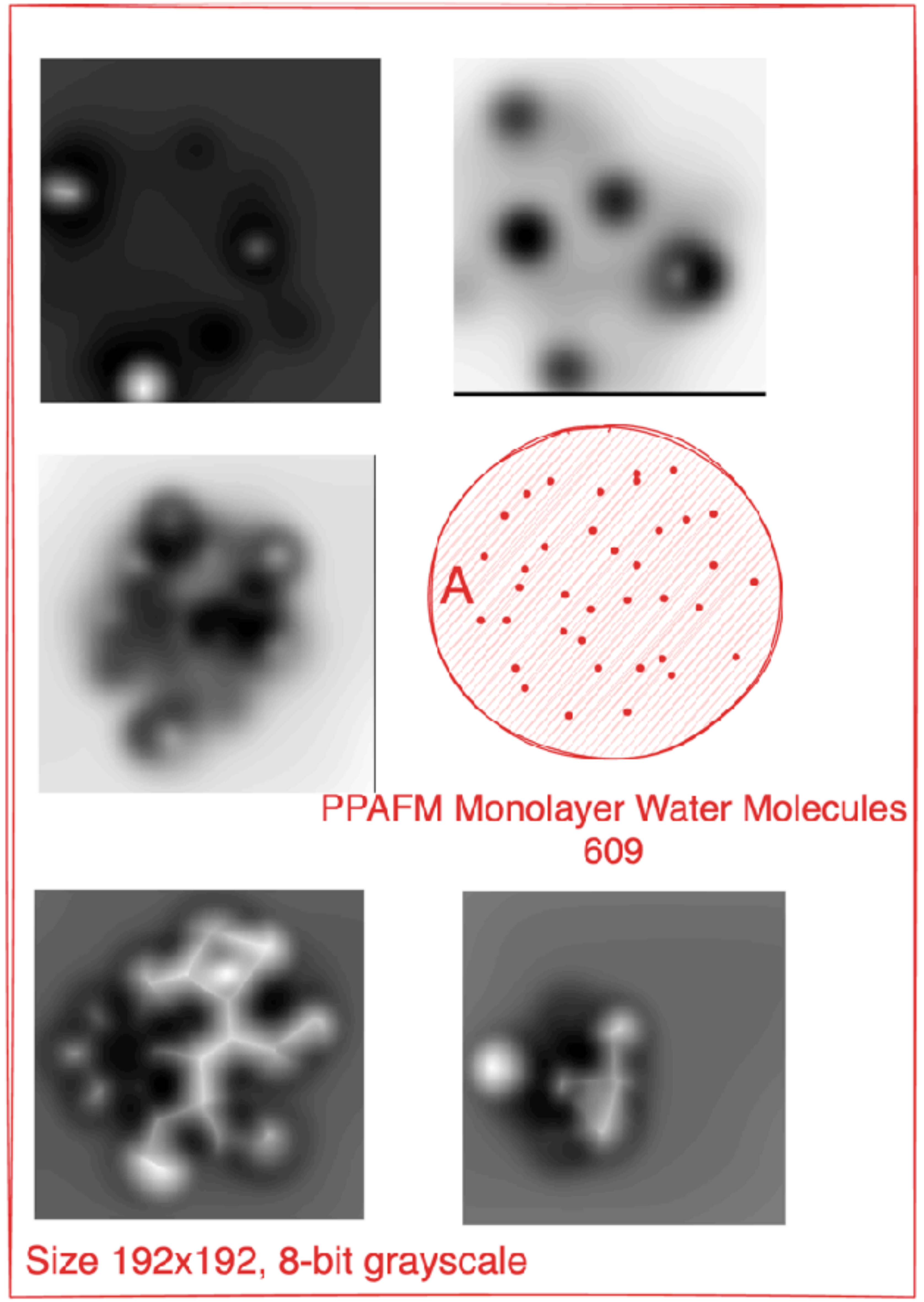
$$\mathcal{L}_{\mathrm{cyc}} = \mathbb{E}_{x \sim p_{\mathrm{data}}(x)}[\|F(G(x)) - x\|_1]$$

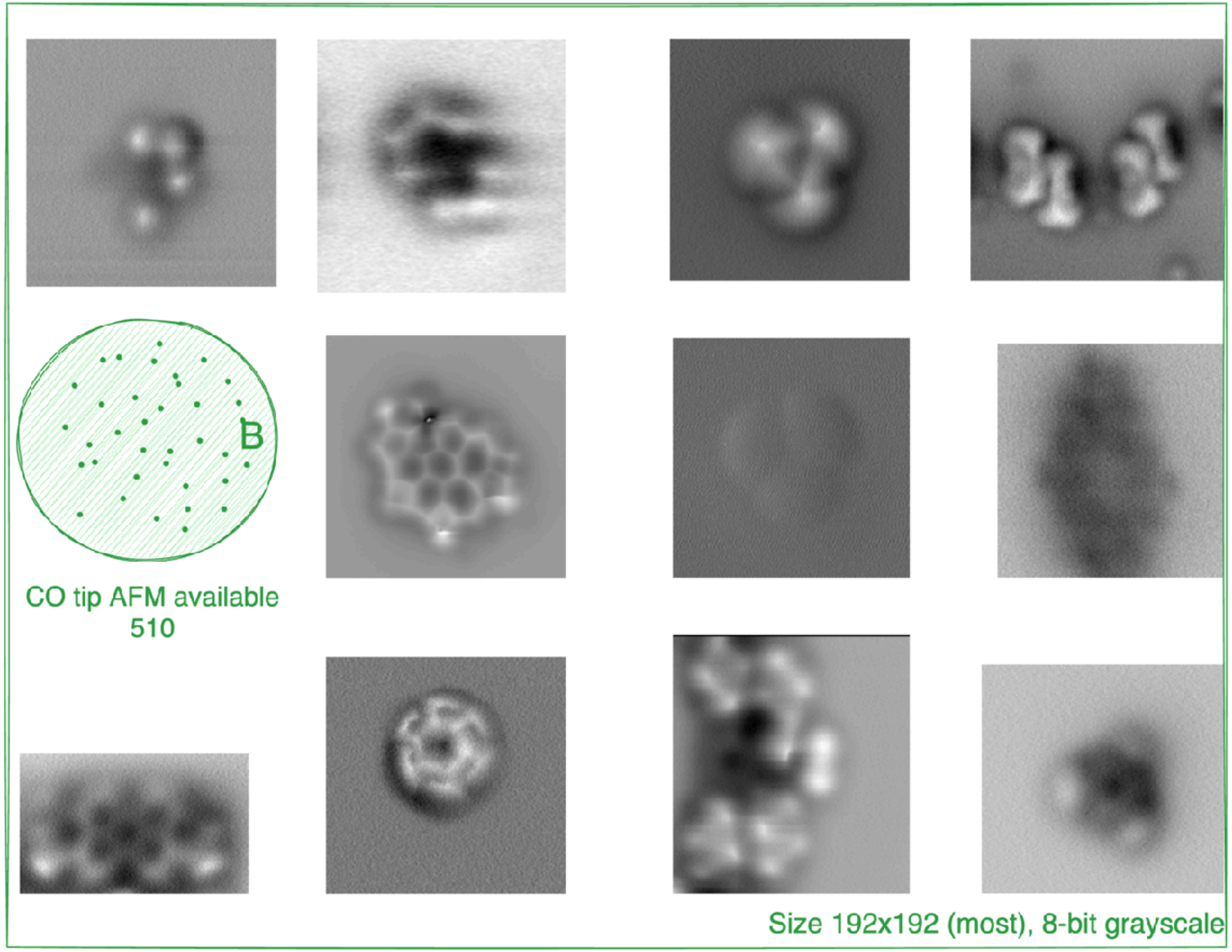
$$\mathcal{L}(G, F, D_X, D_Y) = \mathcal{L}_{\mathrm{GAN}}(G, D_Y, X, Y) + \mathcal{L}_{\mathrm{GAN}}(F, D_X, Y, X) + \lambda \mathcal{L}_{\mathrm{cyc}}(G, F)$$

$$G^*, F^* = \arg\min_{G,F} \max_{D_x, D_Y} \mathcal{L}(G, F, D_X, D_Y)$$

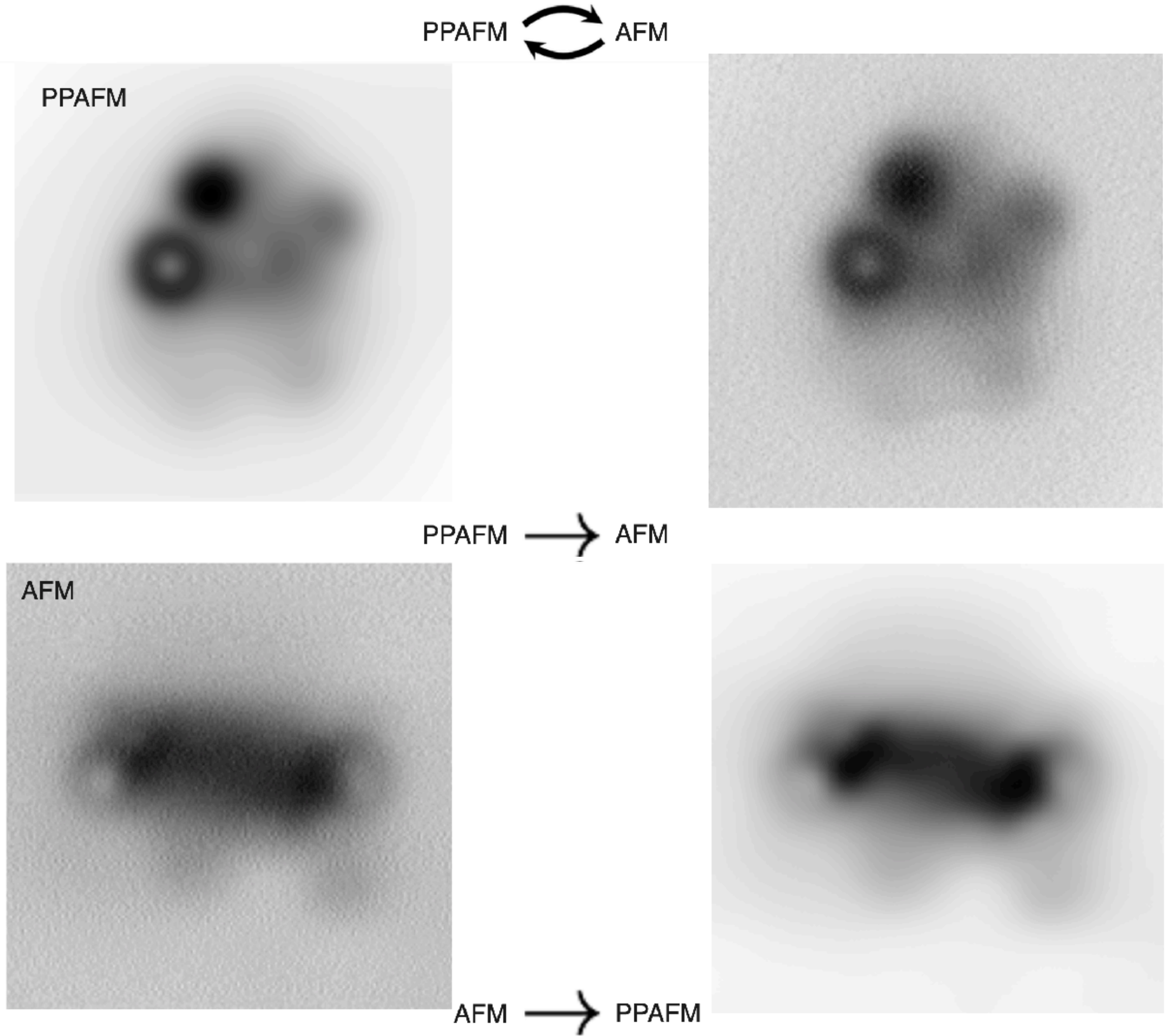


Training samples



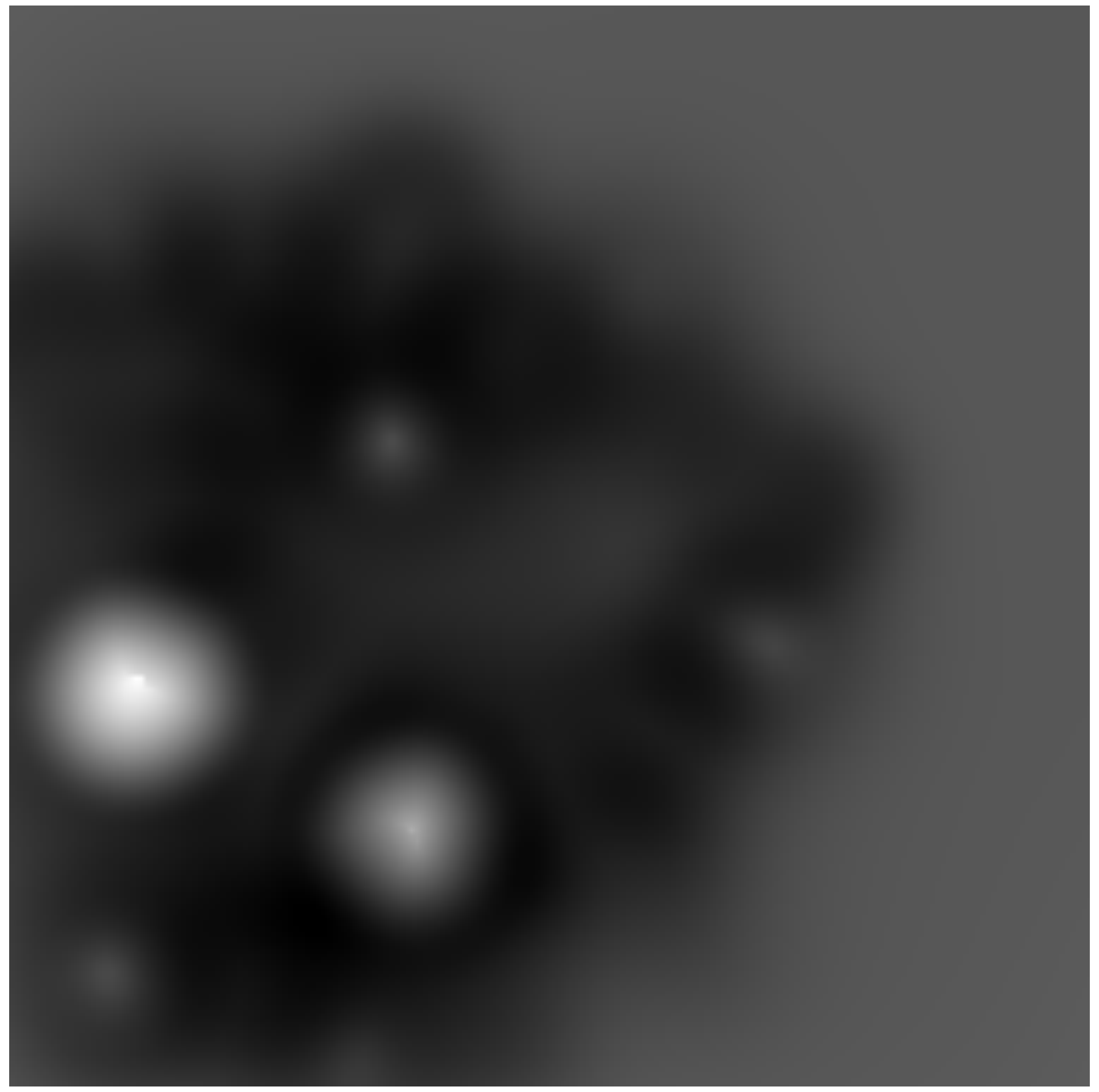


Training Results

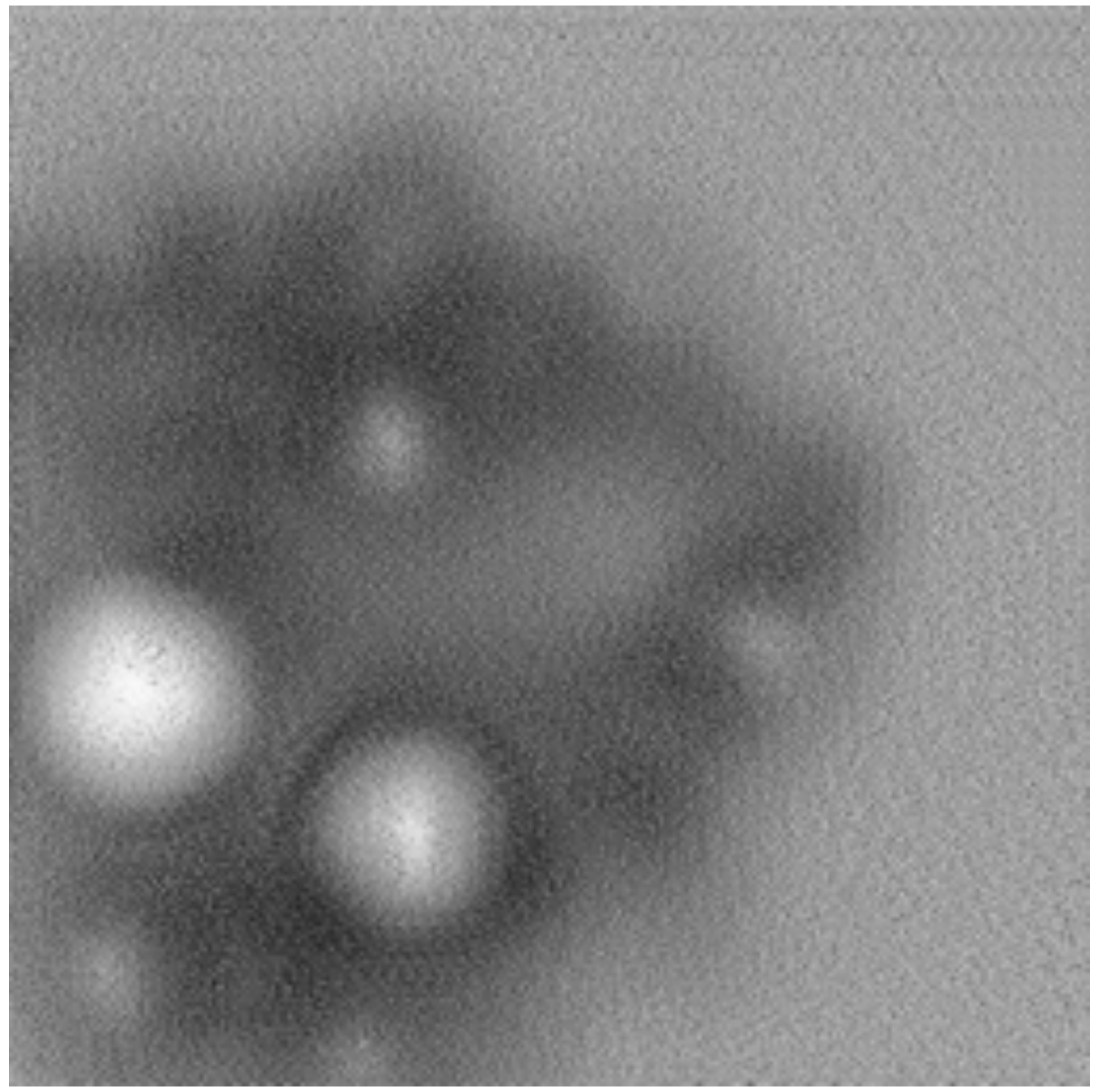


More Translation Examples: A2B

Simulation

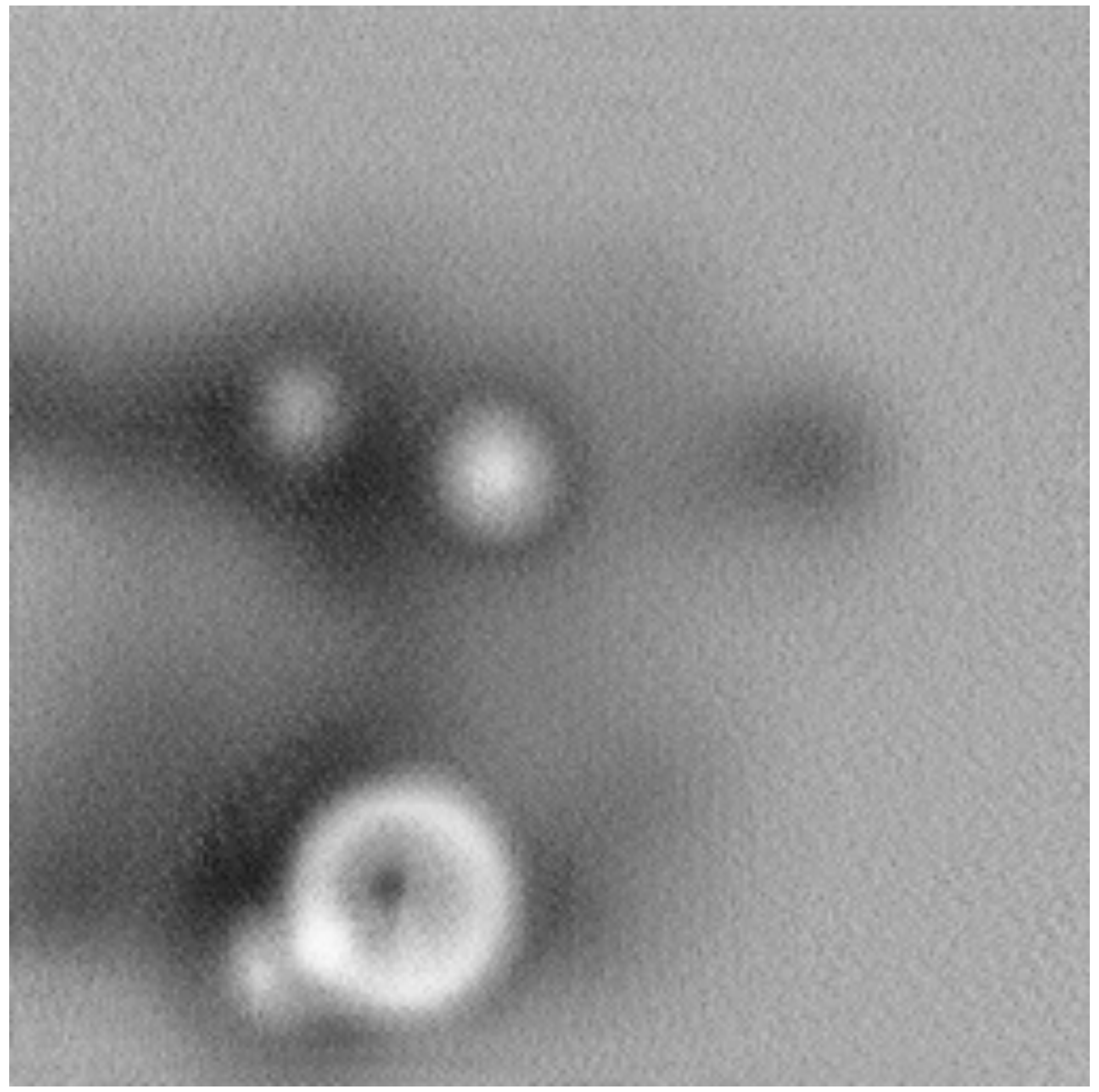


Experimental-style



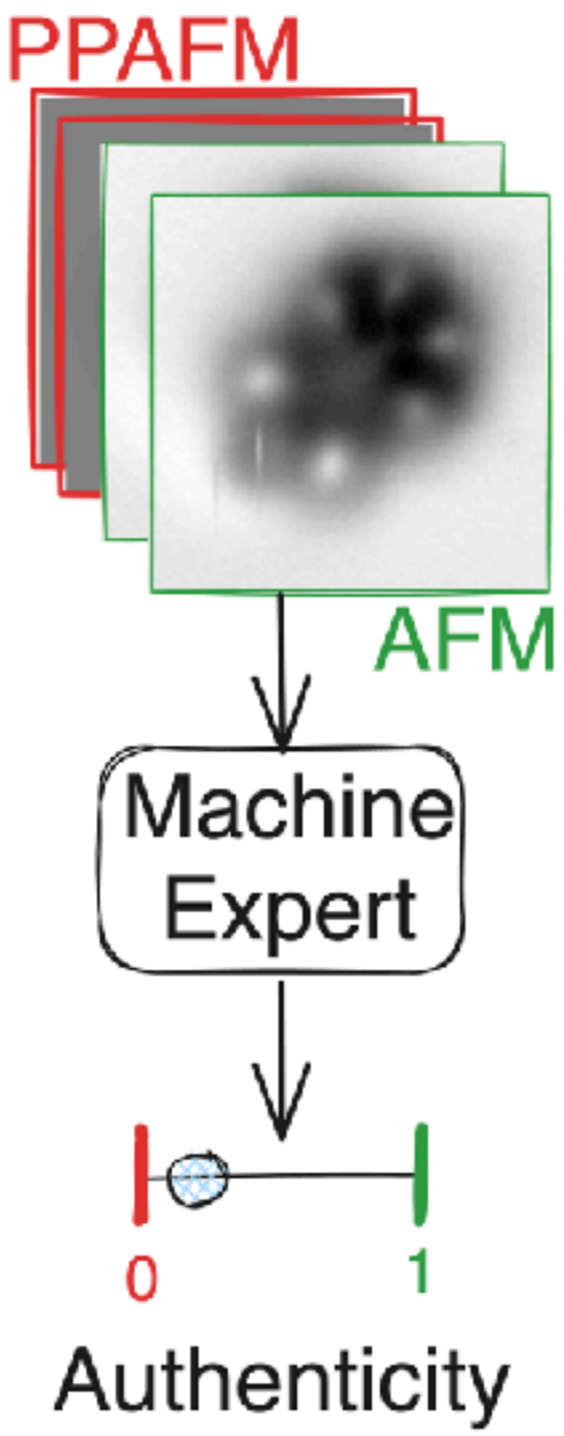
Simulation

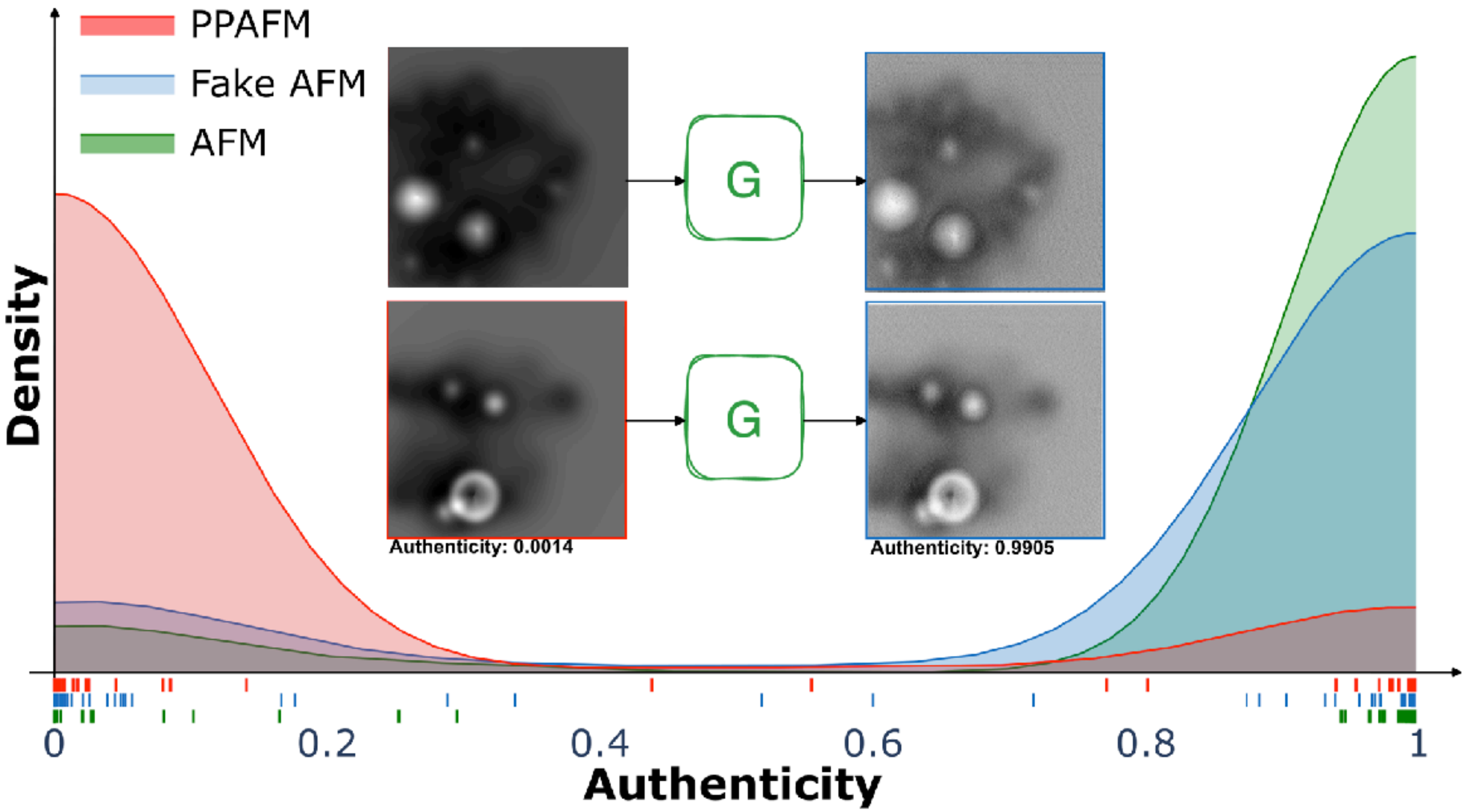
Experimental-style

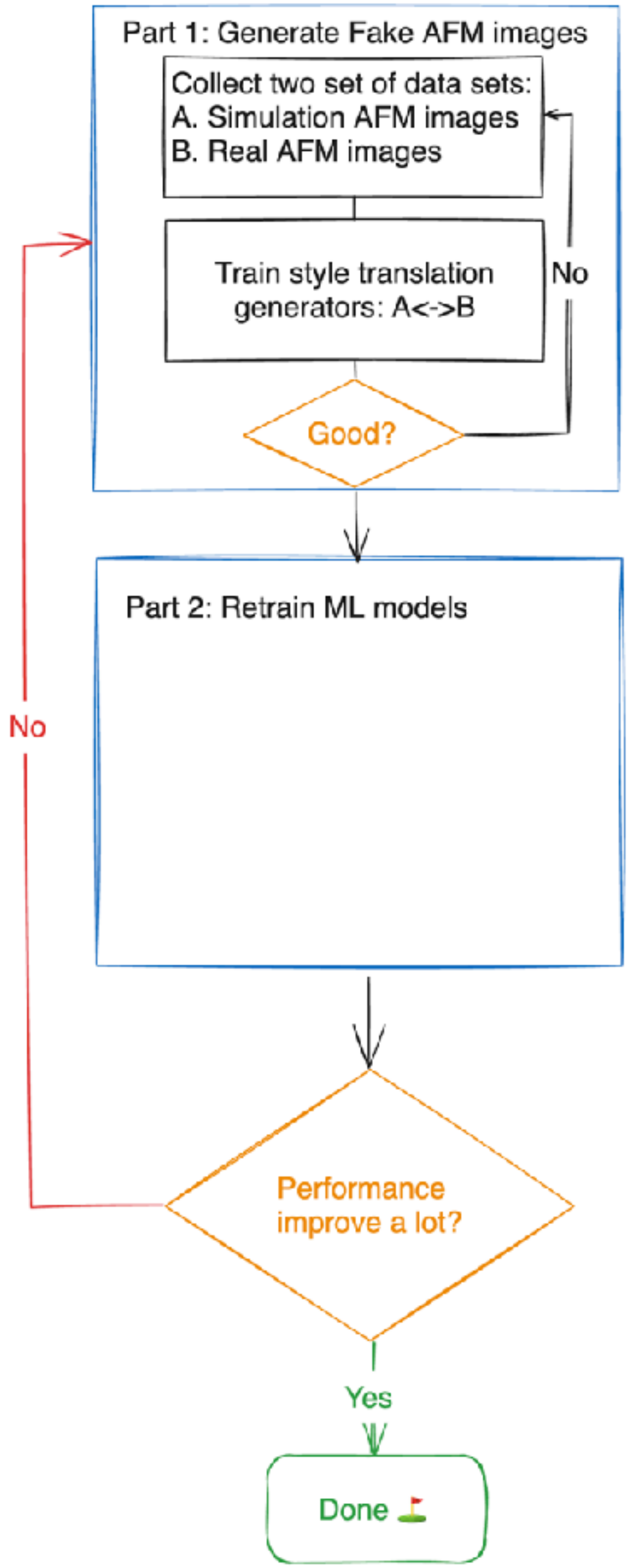


Dataset Evaluation

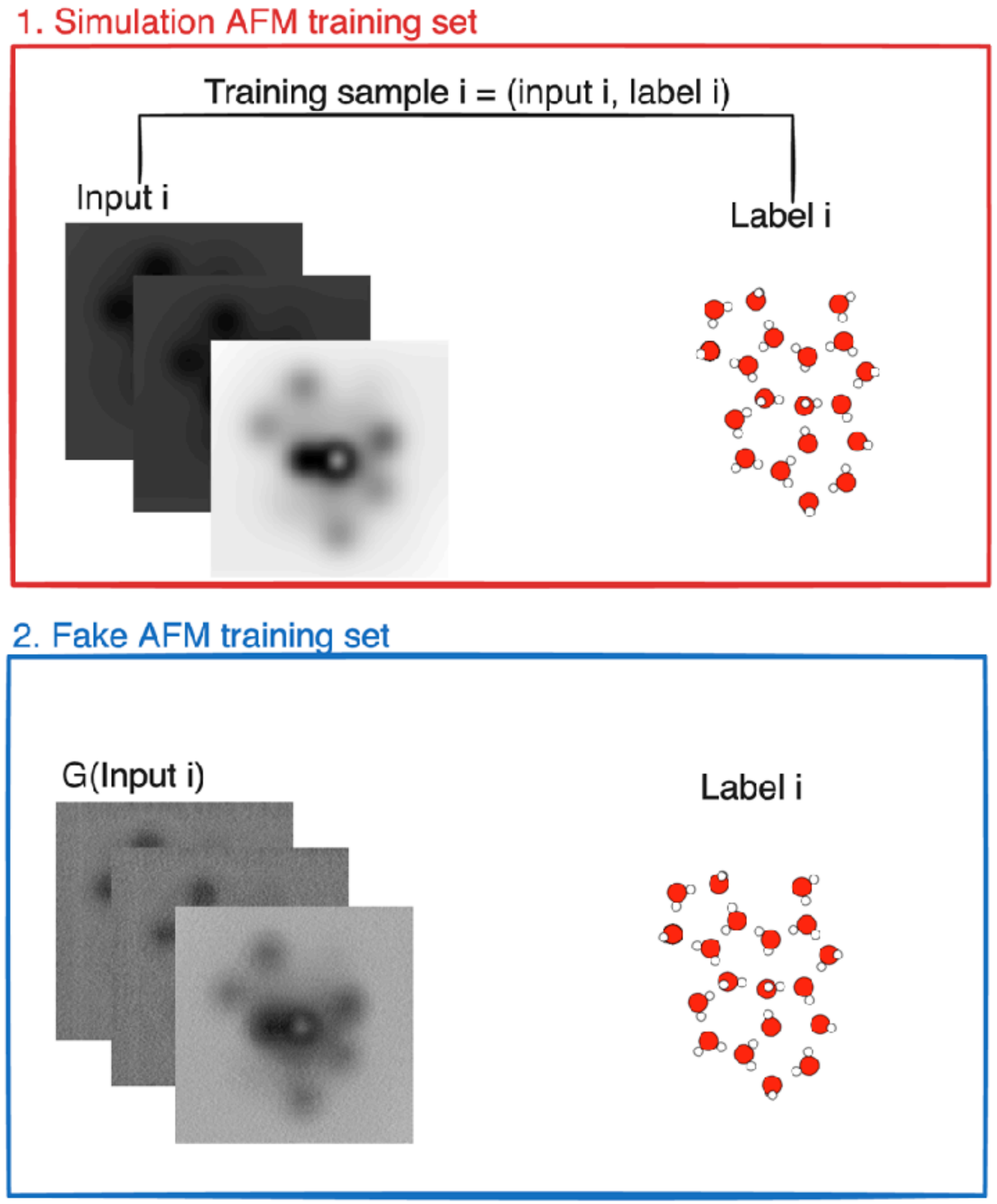
From the perspective of a well trained machine expert.



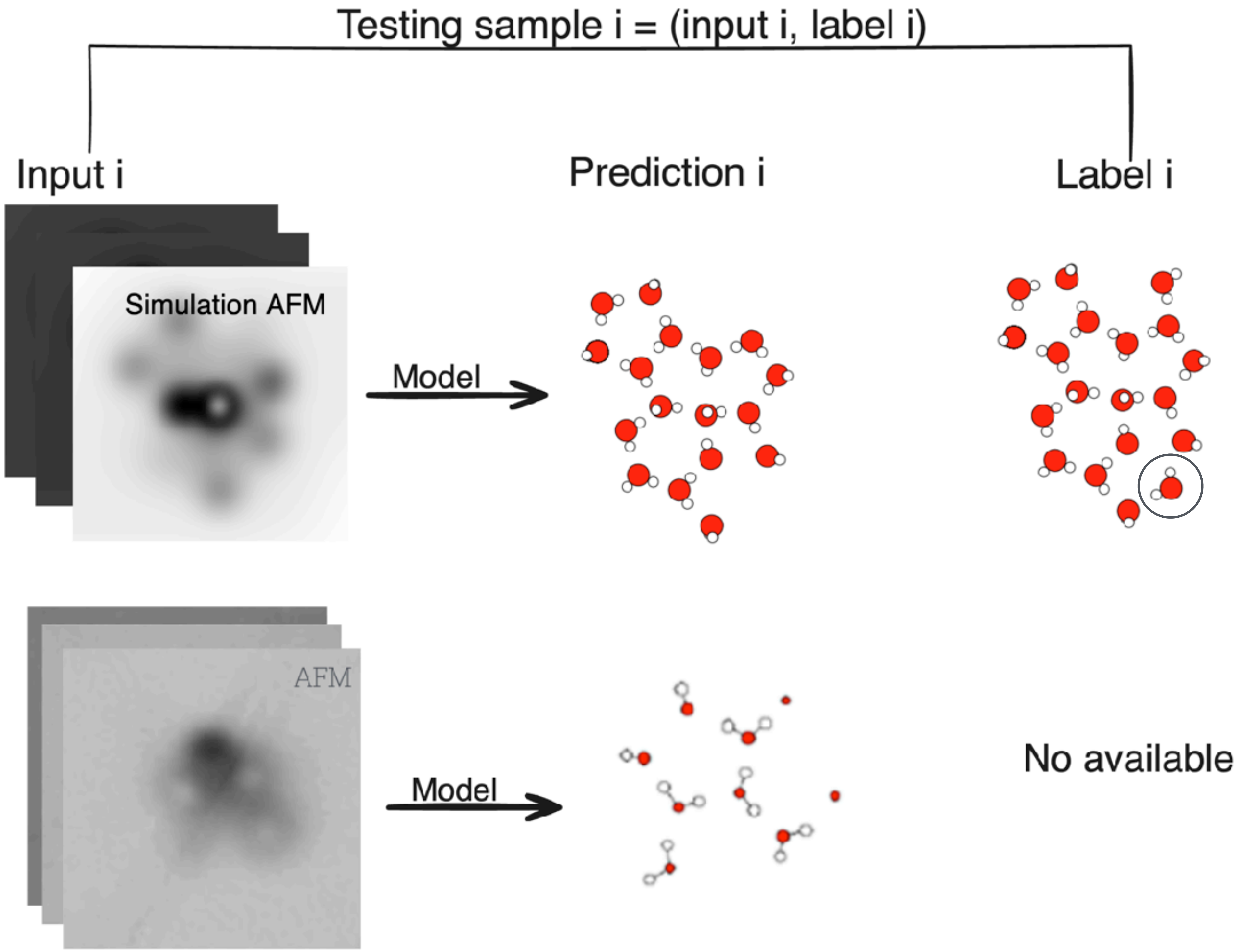




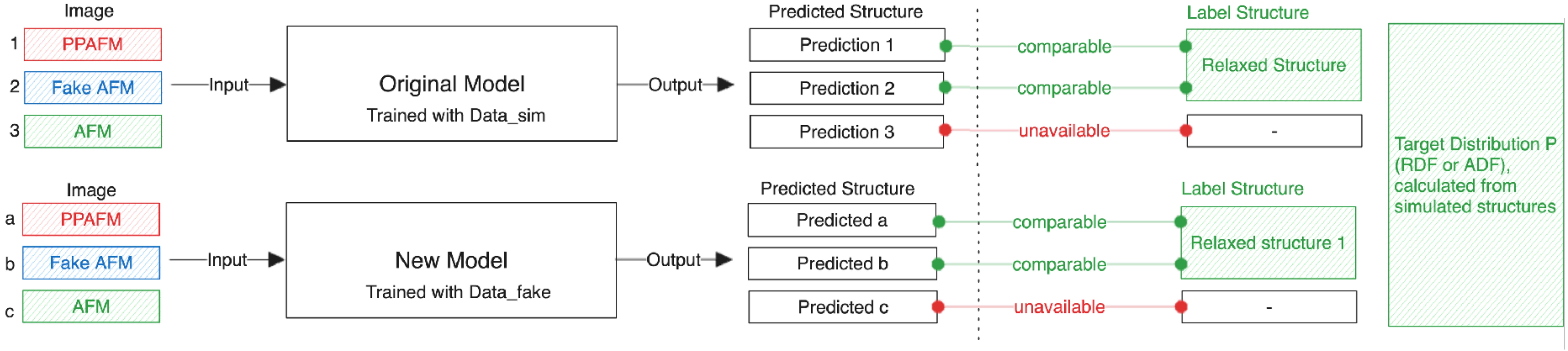
Retrain structure discovery model with different datasets



The challenge of performance evaluation

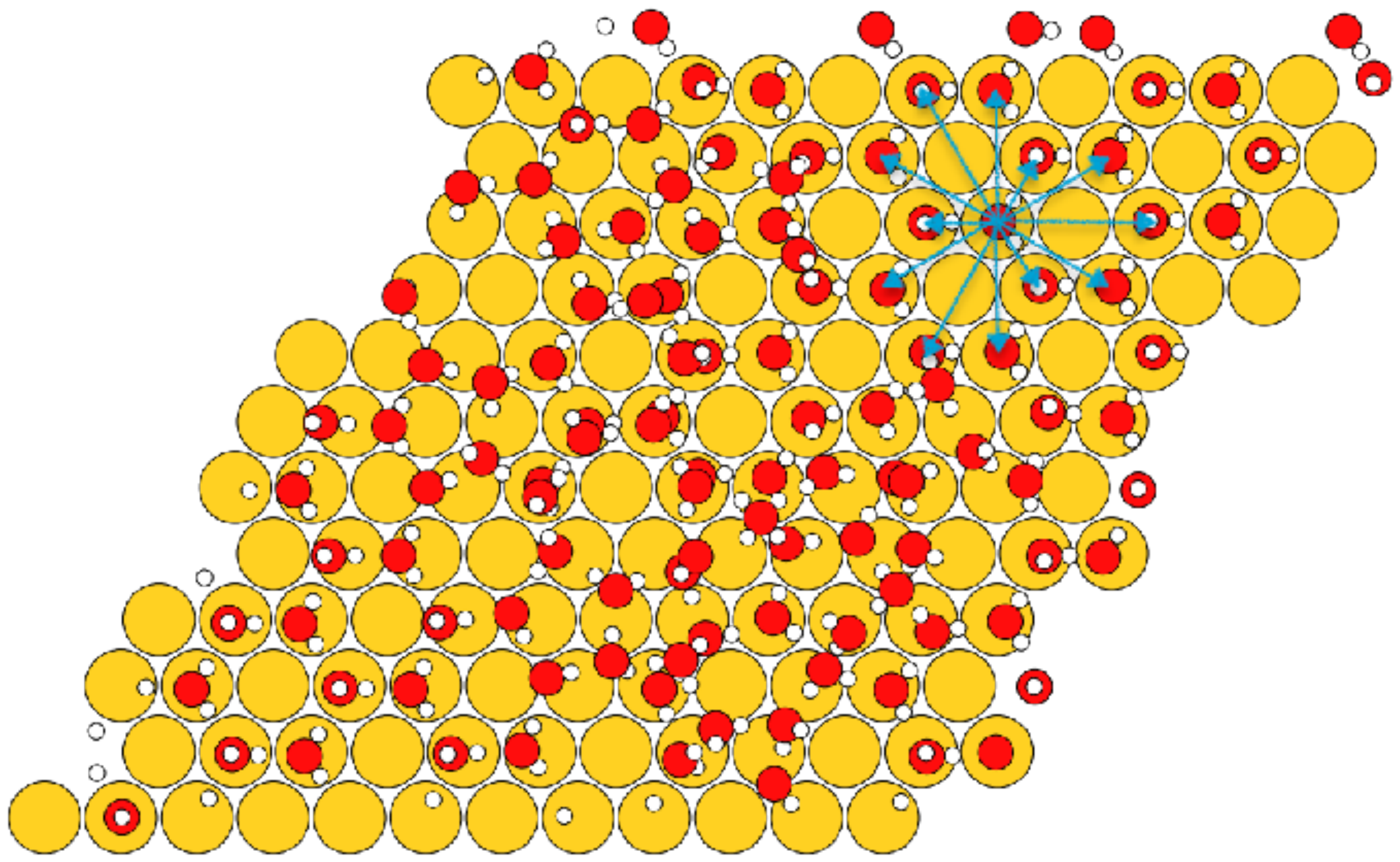


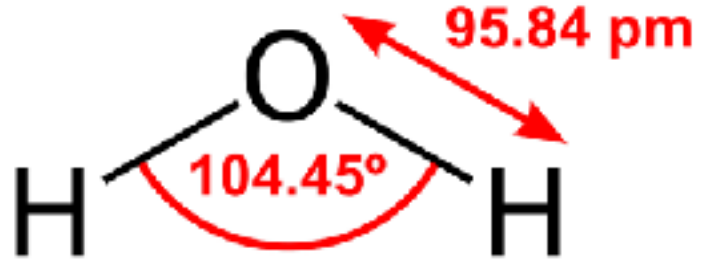
Performance evaluation

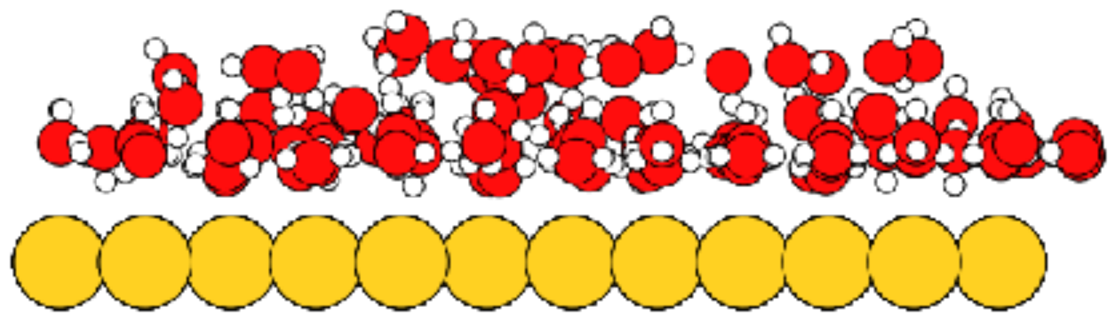


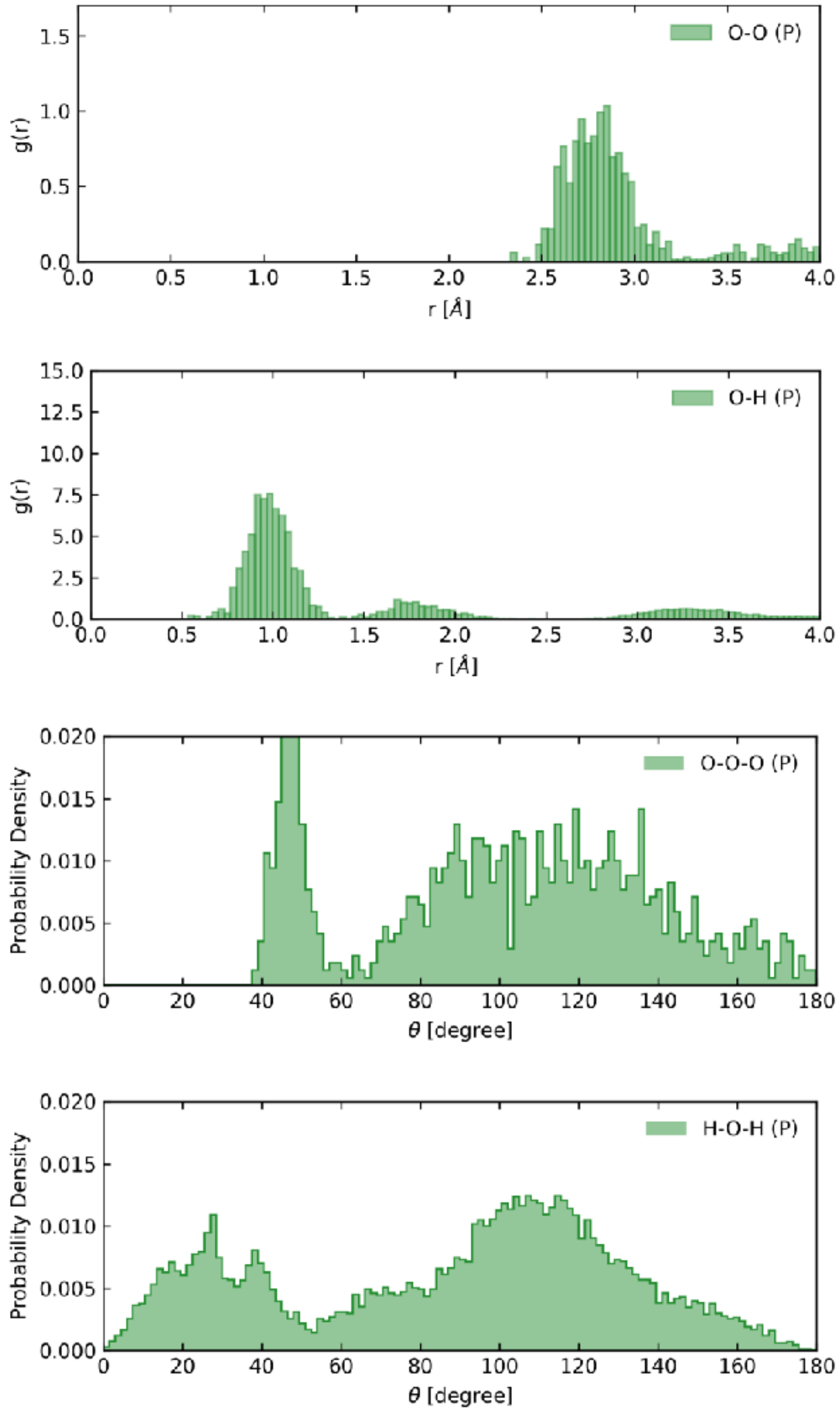
Assumption:
The predicted structure properties (RDF, ADF) on simulation AFM and real AFM are pretty close.

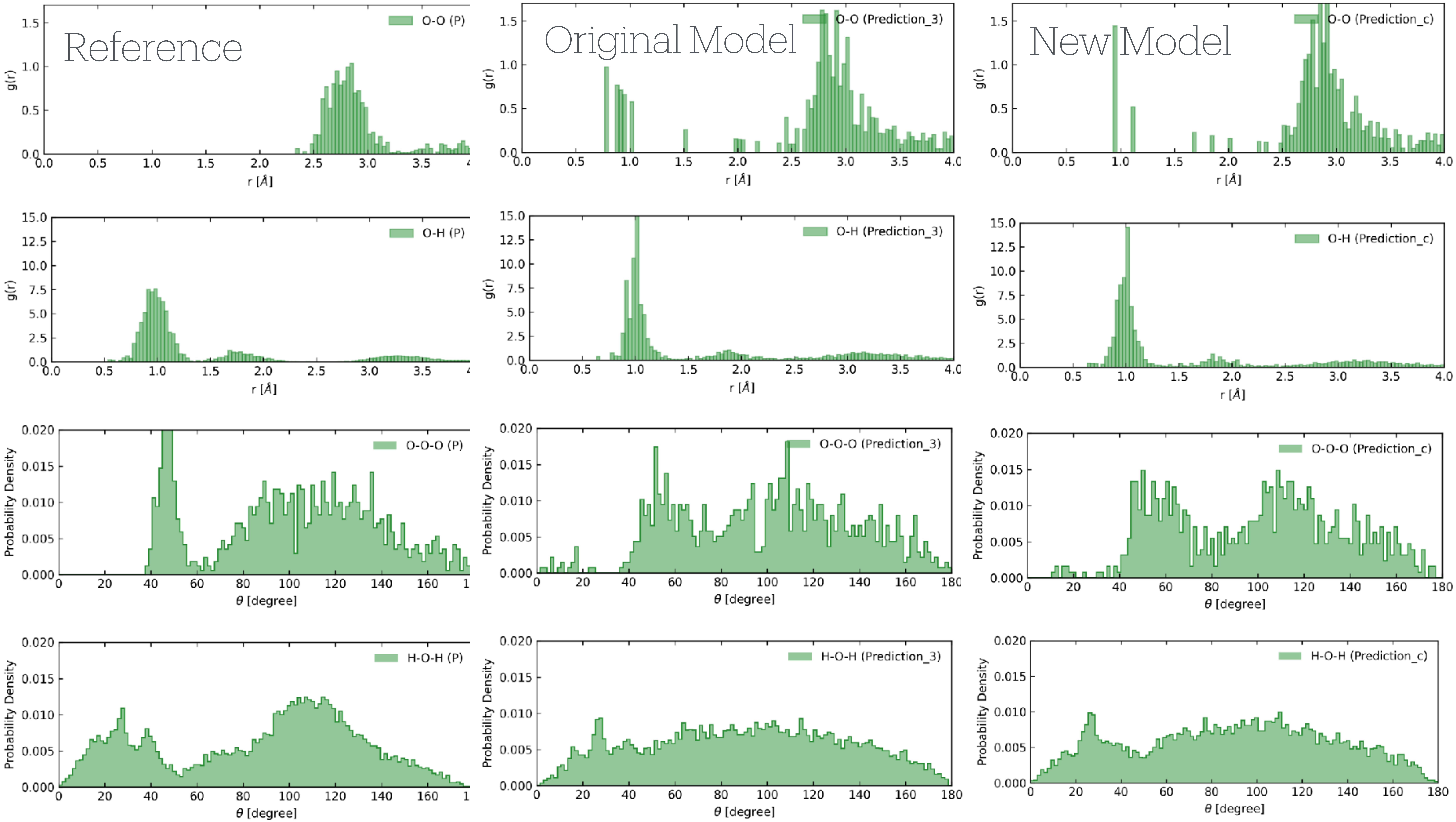
Structure properties: RDF and ADF





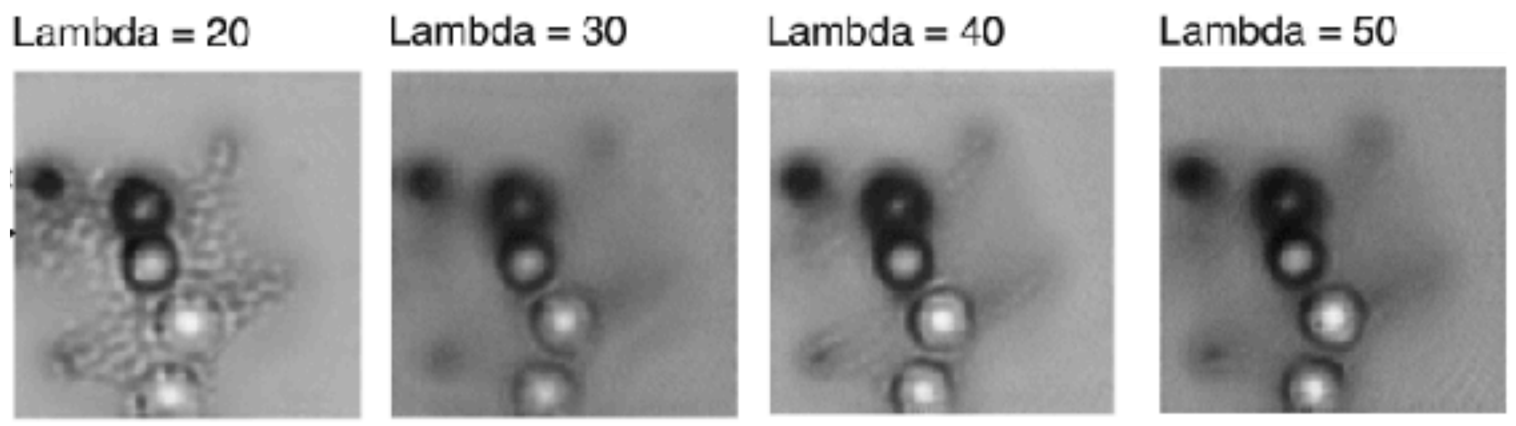




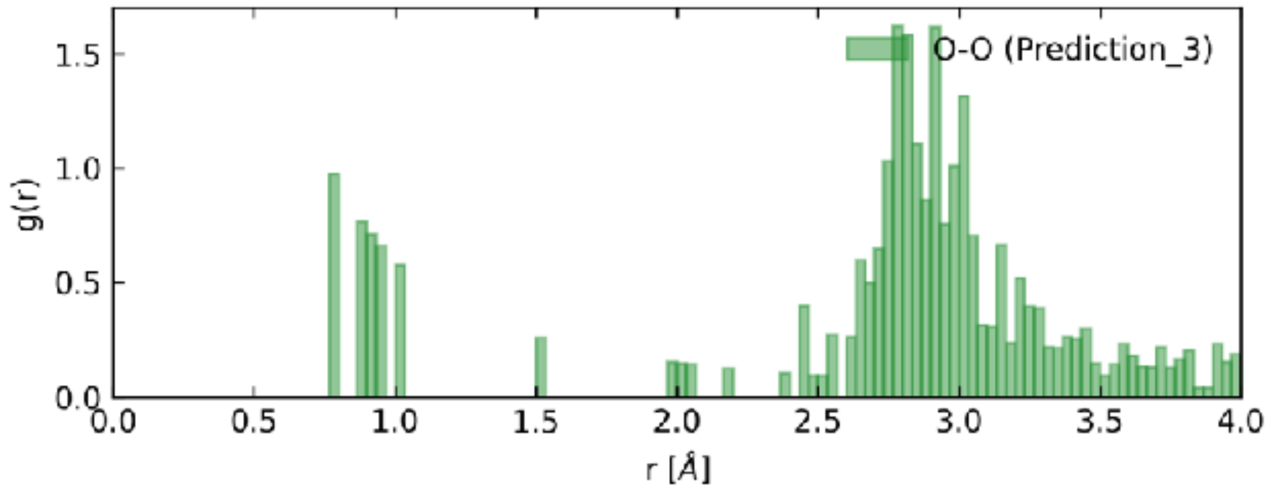

Reference
Original Model
New Model
O-O (P)
O-O (Prediction_3)
O-O (Prediction_c)
O-H (P)
O-H (Prediction_3)
O-H (Prediction_c)
O-O-O (P)
O-O-O (Prediction_3)
O-O-O (Prediction_c)
H-O-H (P)
H-O-H (Prediction_3)
H-O-H (Prediction_c)
g(r)
r [Å]
Probability Density
θ [degree]

Possible reasons and directions

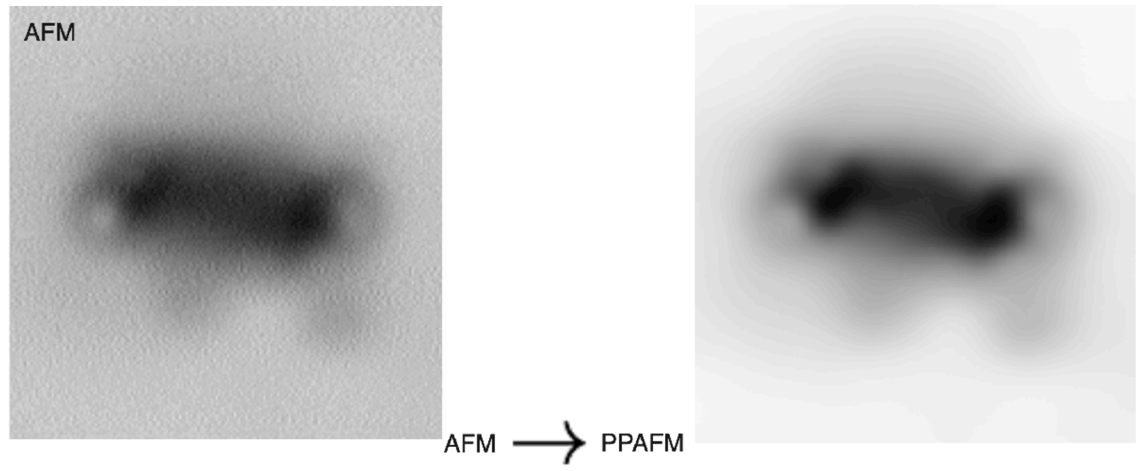
- Hyper-parameter in style translation
  (good in the eyes of human and machine)



- Limitation of data augmentation
  (additional constraint when designing of ML models

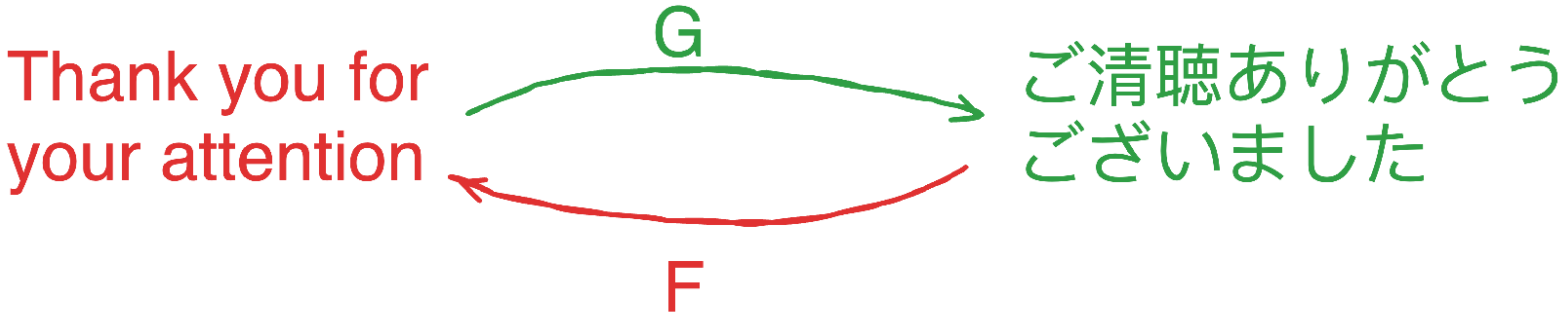


- Using the inverse translation as AFM preprocessing
  (removing is easier than adding, no need to retrain new model)



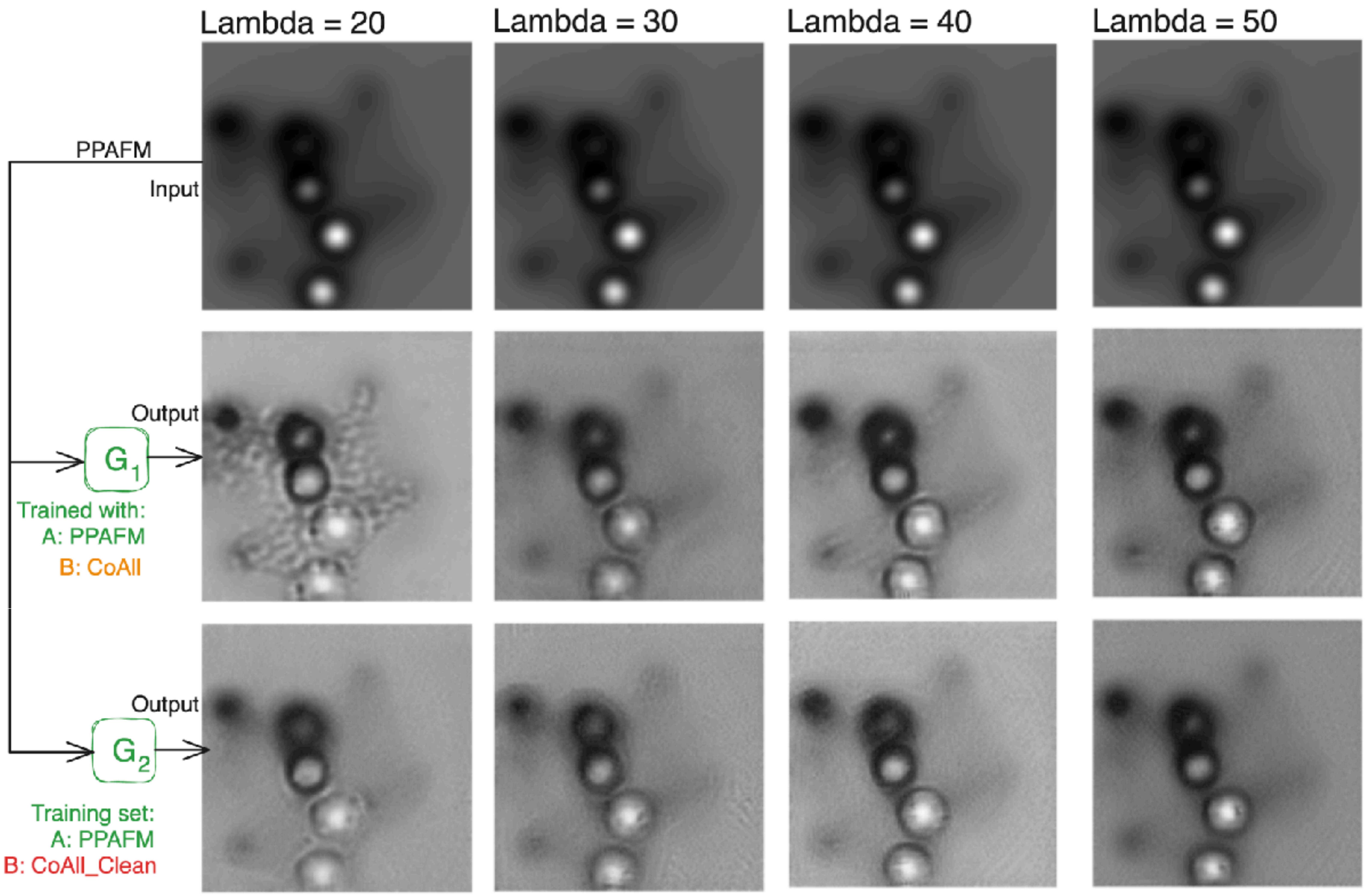
Summary

- CycleGAN provides an effective solution for style translation between simulation and real AFM images.
- Using style translation as a tool of data augmentation is possible. But whether data augmentation can largely improve the performance of ML models is still uncertain.
- The inverse translation from AFM to simulation AFM could be used as an pre-processing (denoising) tool and it's promising to enhance the ML model performance.



Appendix

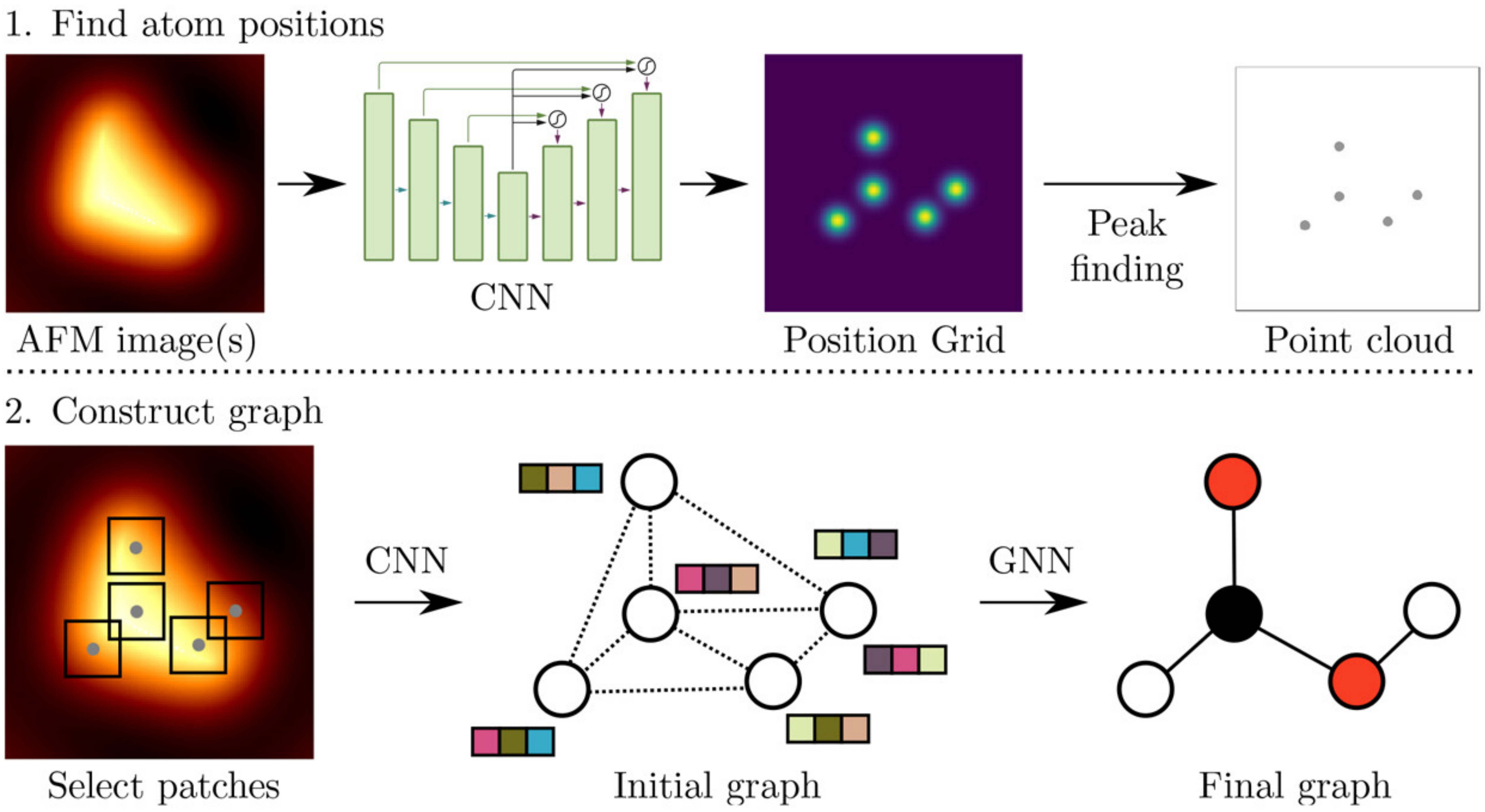
Observations



- Keep model structure simple (less parameters)
- Larger Lambda (L)
- Keep dataset clean

Does the fake AFM dataset good enough?

Appendix



ACS Nano 2024, 18, 7, 5546-5555


Reference
Original Model
New Model
O-O (P)
O-O (Prediction_2)
O-O (Prediction_b)
O-H (P)
O-H (Prediction_2)
O-H (Prediction_b)
O-O-O (P)
O-O-O (Prediction_2)
O-O-O (Prediction_b)
H-O-H (P)
H-O-H (Prediction_2)
H-O-H (Prediction_b)
g(r)
r [Å]
Probability Density
θ [degree]