EXTRACTING QUANTITATIVE DATA FROM STM IMAGES WITH ML

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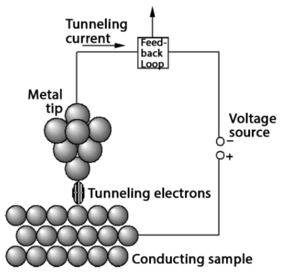
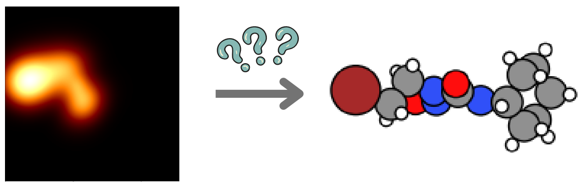
SCANNING TUNNELING MICROSCOPE (STM)

STM works by scanning a sharp conductive probe (tip) very close to the sample surface, then by applying a bias voltage electrons are forced to traverse the gap between them due to the quantum tunneling effect.



The STM image is reconstructed from current variations, revealing atomic-scale features.

Even though novel techniques such as tip functionalization **[1]** have been applied to improve image resolution, interpreting and extracting quantitative data from STM images can still be challenging and time-consuming for researchers.



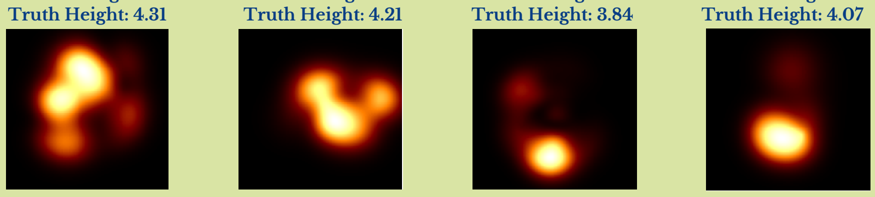
How can we effectively extract quantitive data from STM images using ML ?

MINI PROJECT: STM HEIGHT PREDICTION MODELS

As part of my internship training, we successfully developed two Convolutional Neural Networks (CNN)-based models for predicting the height of STM images.

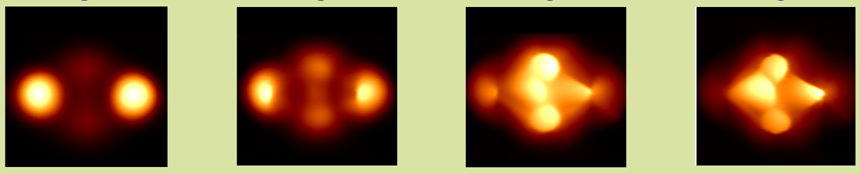
Both models performed well in accurately predicting for simulated STM images:

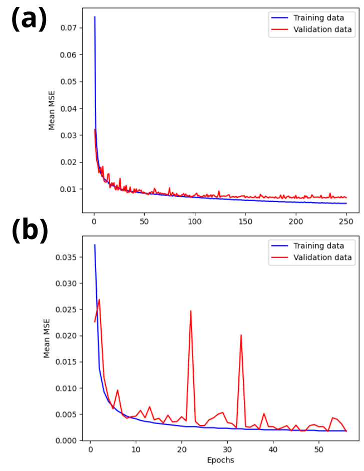
Predicted Height: 4.30 Truth Height: 4.31	Predicted Height: 4.20 Truth Height: 4.21	Predicted Height: 3.80 Truth Height: 3.84	Predicted Height: 4.10 Truth Height: 4.07



However, when the models were applied to experimental images, the predictions from both models (a) & (b) were not sufficiently reliable but model (b) exhibited better performance:

Pred. Height: 3.005	Pred. Height: 3.029	Pred. Height: 2.936	Pred. Height: 2.701

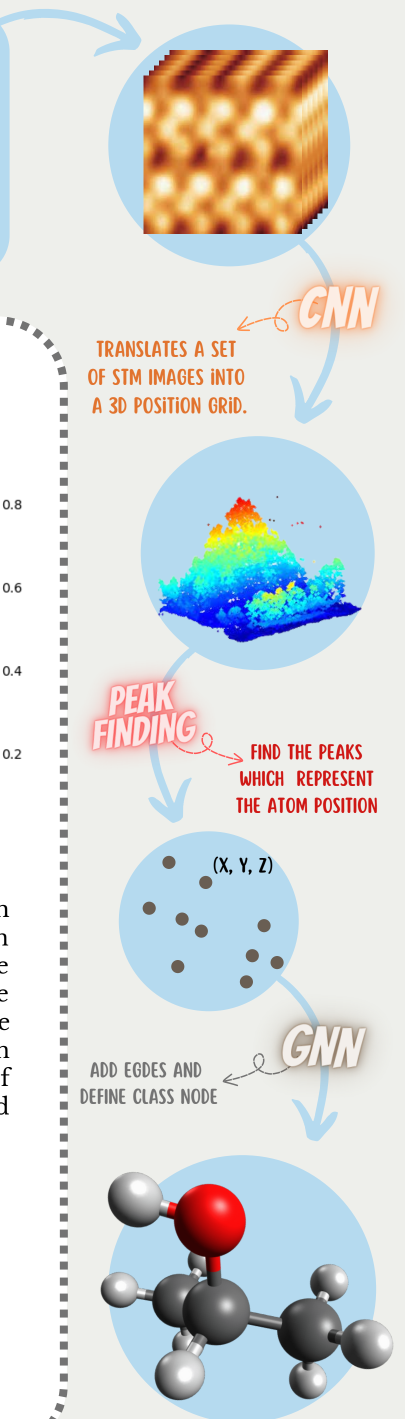




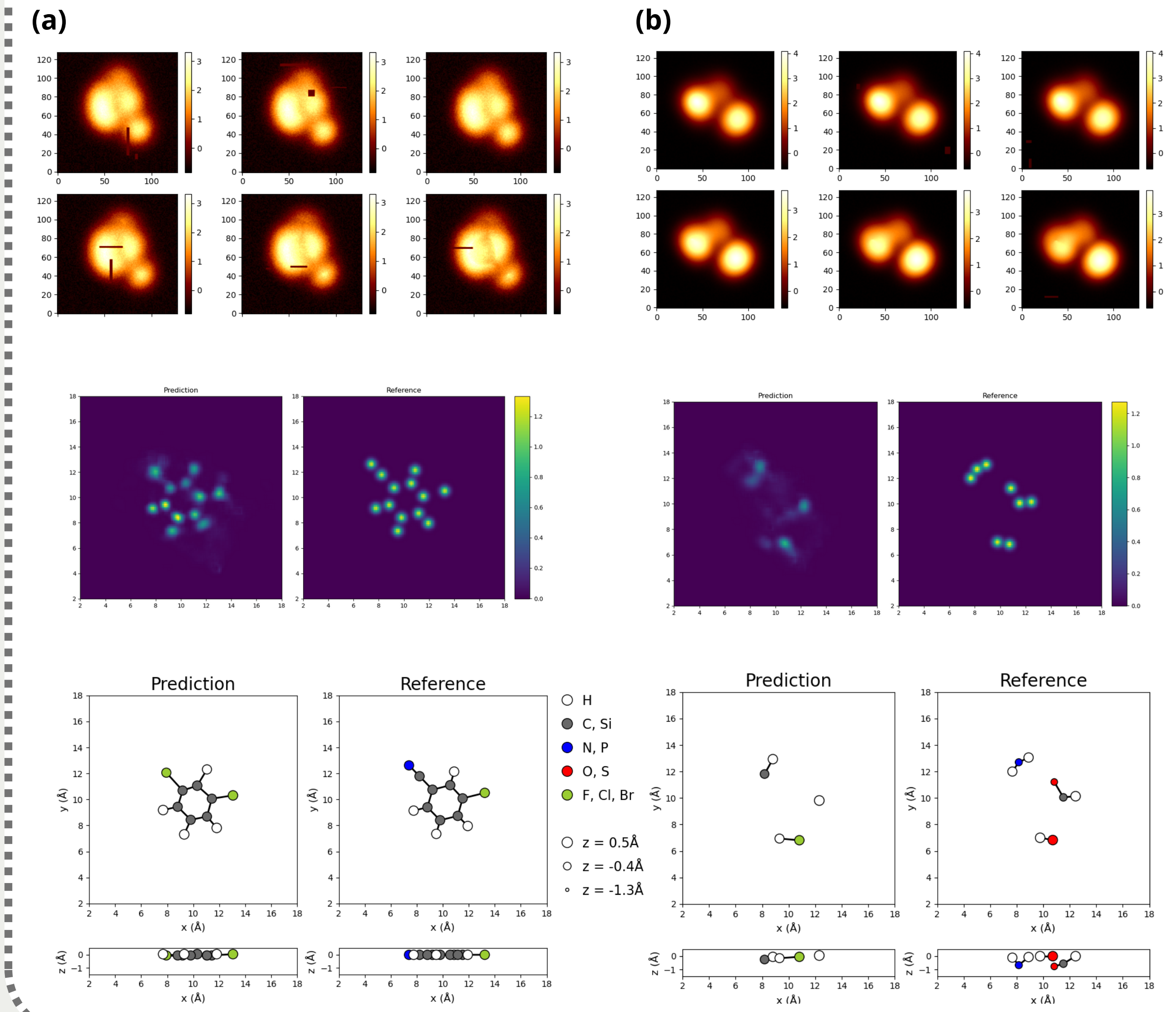
Mean MSE vs Epochs of model **(a)** and **(b)**, where the second model converged to less error in fewer epochs.

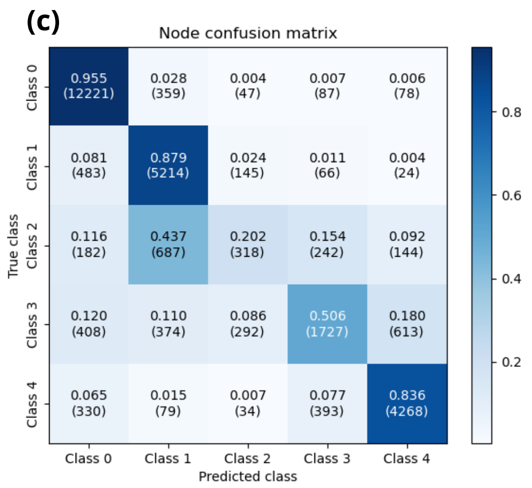
GRAPH RECONSTRUCTION MODEL

The model architecture used in this project was developed by **[2]**. It consisted by a U-net type CNN with attention gates, followed by a peak finding algorithm, where we are able to extract the atom positions. The next step is to construct a graph by finding the atom class and edge, this is achieved by using a Graph Neural Network (GNN), adding one node at a time to the graph.



GRAPH RECONSTRUCTION RESULTS





True class \ Predicted class	Class 0	Class 1	Class 2	Class 3	Class 4
Class 0	0.955 (12221)	0.028 (359)	0.004 (47)	0.007 (87)	0.006 (78)
Class 1	0.081 (483)	0.879 (5214)	0.024 (145)	0.011 (66)	0.004 (24)
Class 2	0.116 (182)	0.437 (687)	0.202 (318)	0.154 (242)	0.092 (144)
Class 3	0.120 (408)	0.110 (374)	0.086 (292)	0.506 (1727)	0.180 (613)
Class 4	0.065 (330)	0.015 (79)	0.007 (34)	0.077 (393)	0.836 (4268)

(a), (b) Graph predictions from simulated STM images. **(c)** Confusion Matrix of atom classification. The values have been normalized by the total number of true cases of the corresponding class, and the values in parenthesis show the total number of cases with the corresponding true and predicted class.

MORE RESULTS? EXPLORE THEM HERE

MORE PROJECTS? SIN GROUP GITHUB

REFERENCES

[1] Krejčí, O., Hapala, P., Ondráček, M., & Jelínek, P. (2017). Principles and simulations of high-resolution STM imaging with a flexible tip apex. Physical Review B, 95(4), 045407.

[2] Oinonen, N., Kurki, L., Ilin, A. et al. Molecule graph reconstruction from atomic force microscope images with machine learning. MRS Bulletin 47, 895–905 (2022).

[3] Alldritt, B., Hapala, P., Oinonen, N., Urtev, F., Krejci, O., Federici Canova, F., ... & Foster, A. S. (2020). Automated structure discovery in atomic force microscopy. Science advances, 6(9), eaay6913.

CONCLUSIONS

- The height prediction models worked reliably for simulated STM images but were less effective with experimental ones. We observed a sequential pattern from lower to higher heights in the experimental images, leading us to conclude that the second model performed better. Further improvements are required to enhance accuracy with real-world experimental data.
- Regarding the graph reconstruction model, the CNN part works well for predicting atom positions, but it still has room for improvement, as it occasionally misses some atom positions.
- The confusion matrix of the graph model revealed difficulties in predicting atoms of "class 2" (N and P) and "class 3" (O and S).
- Graph model [1] have shown promise for interpreting STM & AFM images, but refinement is needed to enhance reliability, and also needs to incorporate a wider variety of atoms for a general use.

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