Automated Structure Discovery in Atomic Force Microscopy

Benjamin Alldritt[1], Prokop Hapala[1], Fedor Urtev[1], Niko Oinonen[1], Ondrej Krejčí[1], Filippo Federici Canova[1,3], Fabian Schultz[4], Juho Kannala[2], Peter Liljeroth[1], Adam Foster[1,5,6]

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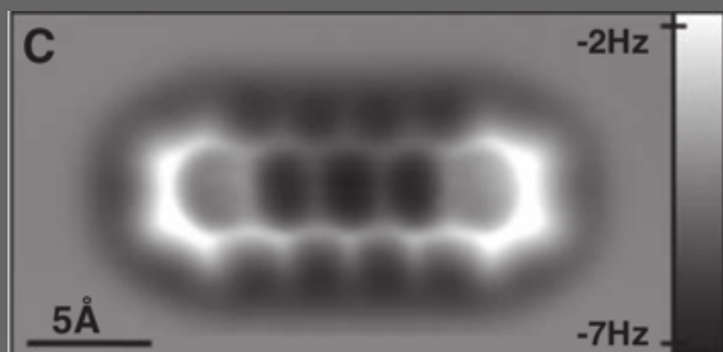
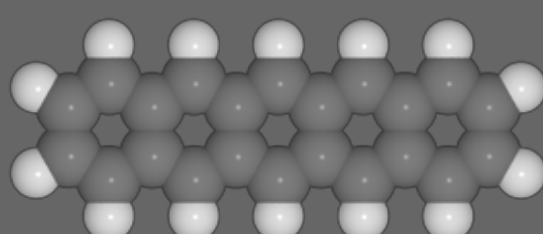
[1]Department of Applied Physics, Aalto University, P.O. Box 11100, 00076 Aalto, Espoo, Finland
[2]Department of Computer Science, Aalto University, P.O. Box 11100, 00076 Aalto, Espoo, Finland
[3]Nanolayers Research Computing Ltd, London, UK
[4]BM Research-Zurich, Säumerstrasse 4, 8803 Rüschlikon, Switzerland
[5]Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128, Germany
[6]WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University , Kakuma-machi, Kanazawa 920-1192, Japan

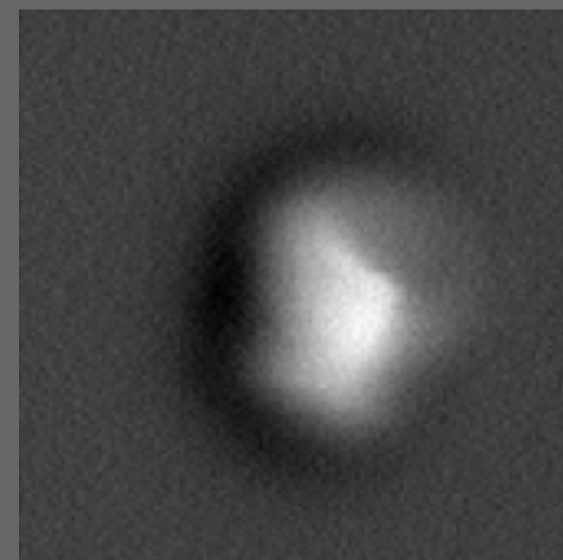
What is this about?

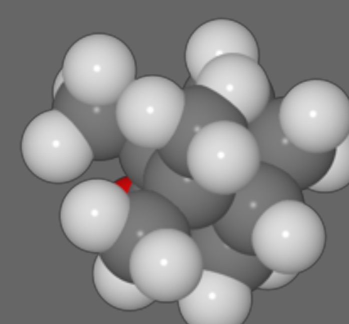
What is this?

That's pentacene





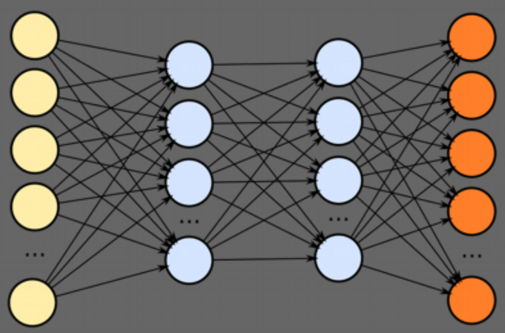




Gross et al. (2009)

Advances in deep learning

Artificial neural network



- Computer vision
- Language processing
- Playing Games
- ...

Machine translation

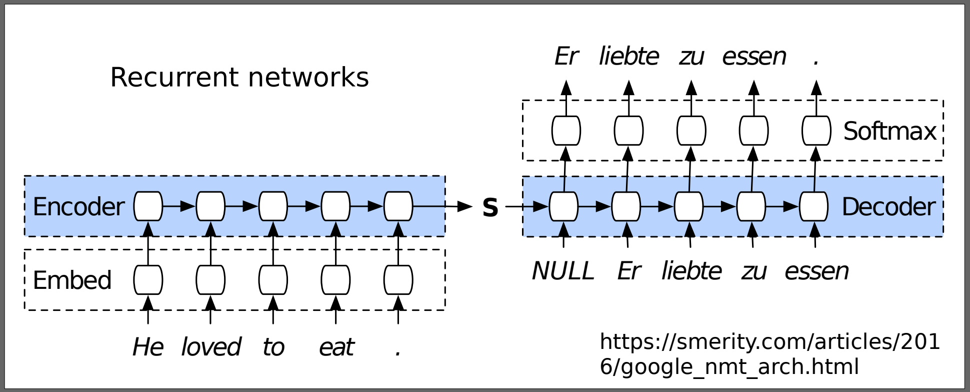
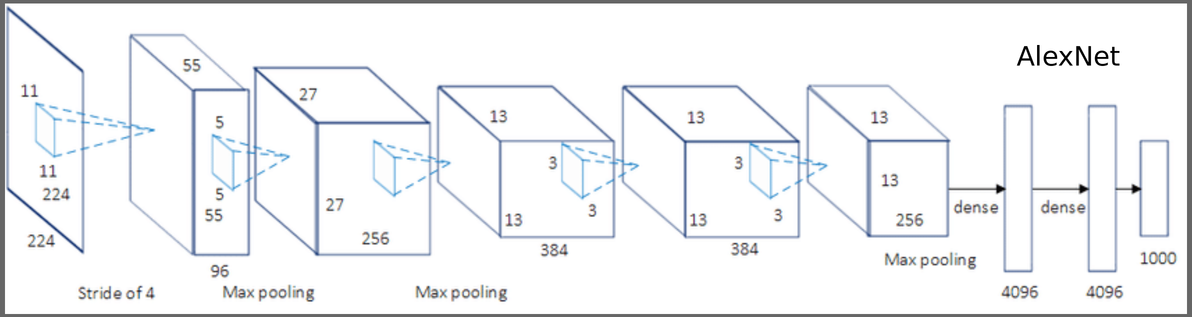


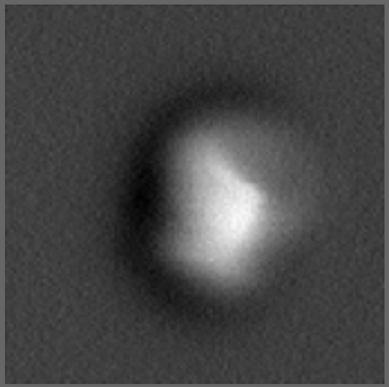
Image recognition

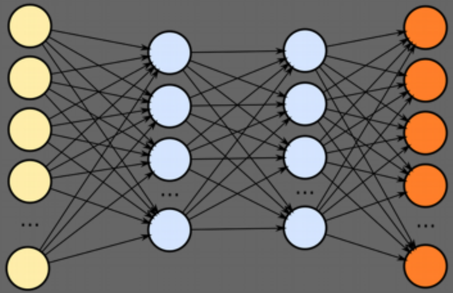


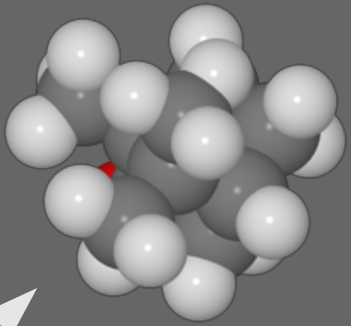
It's a dog

Goal

AFM + Deep Learning = Win?

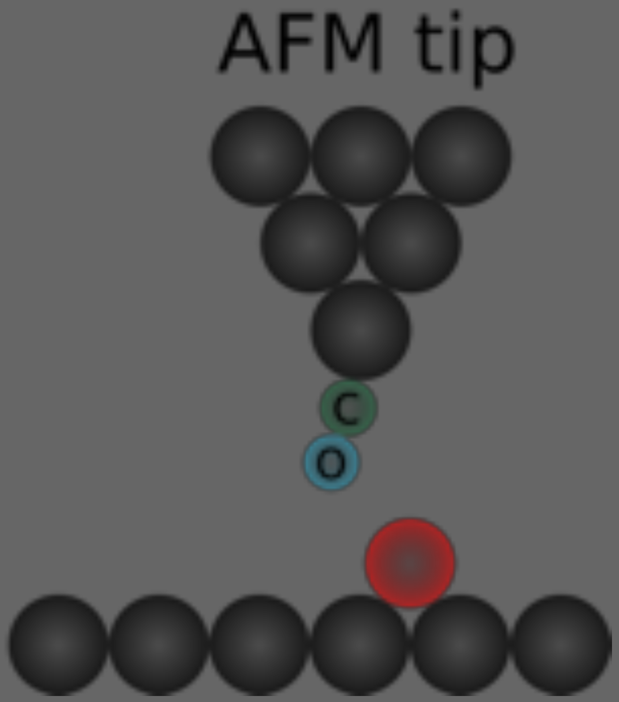




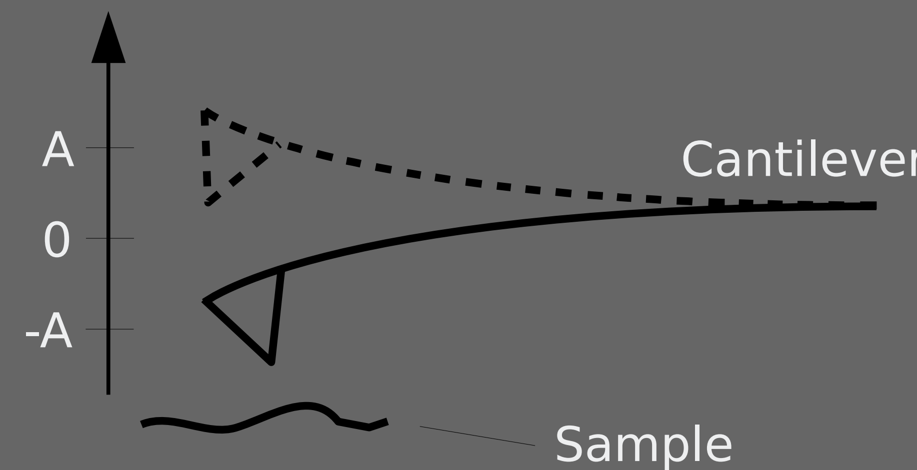


Spatial structure,
Chemical properties,
Which molecule?

Atomic force microscopy (AFM)

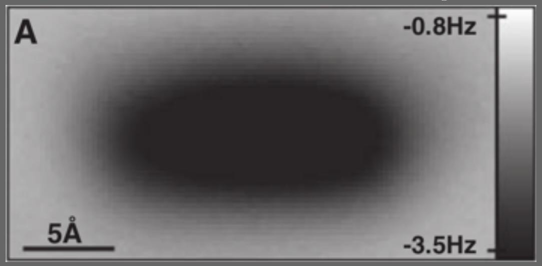


https://commons.wikimedia.org/wiki/File:AFM_tip_with_CO-functionalization.png

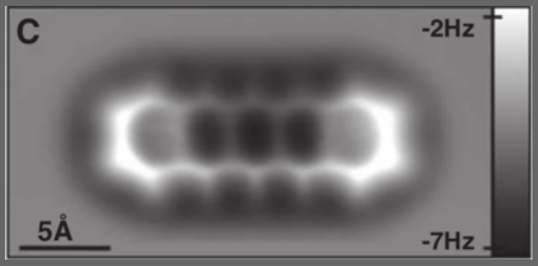


- FM-AFM: drive cantilever at resonance, measure frequency shift **Δf**
- Tip functionalization: CO, Cl, Xe, etc.

Bare metallic tip:



CO-functionalized tip:



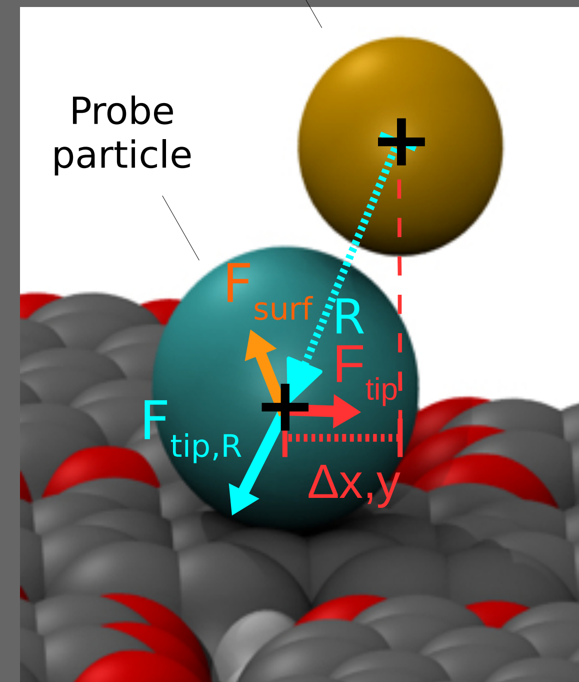
Gross et al. (2009)

Probe particle model

- Lennard-Jones + electrostatics + spring force
- Efficient GPU implementation

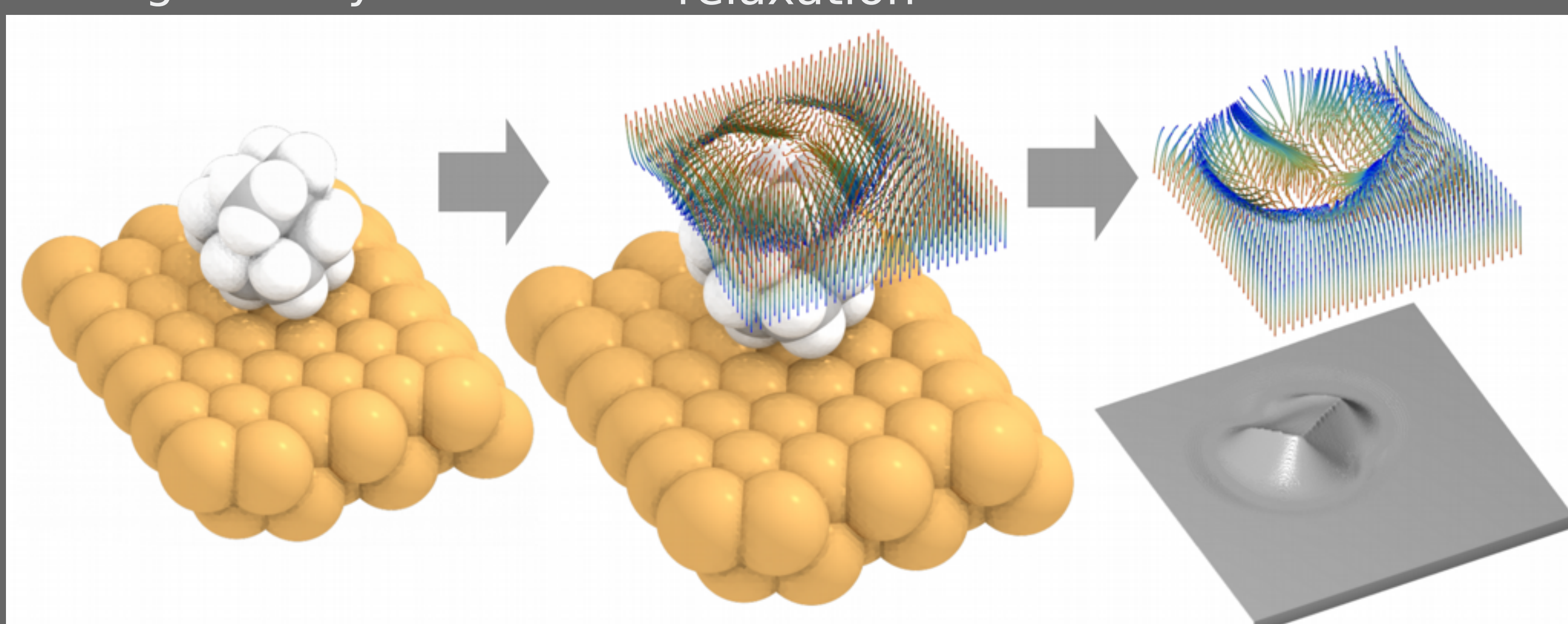
  → ~50 simulations/second

Tip



Molecular geometry

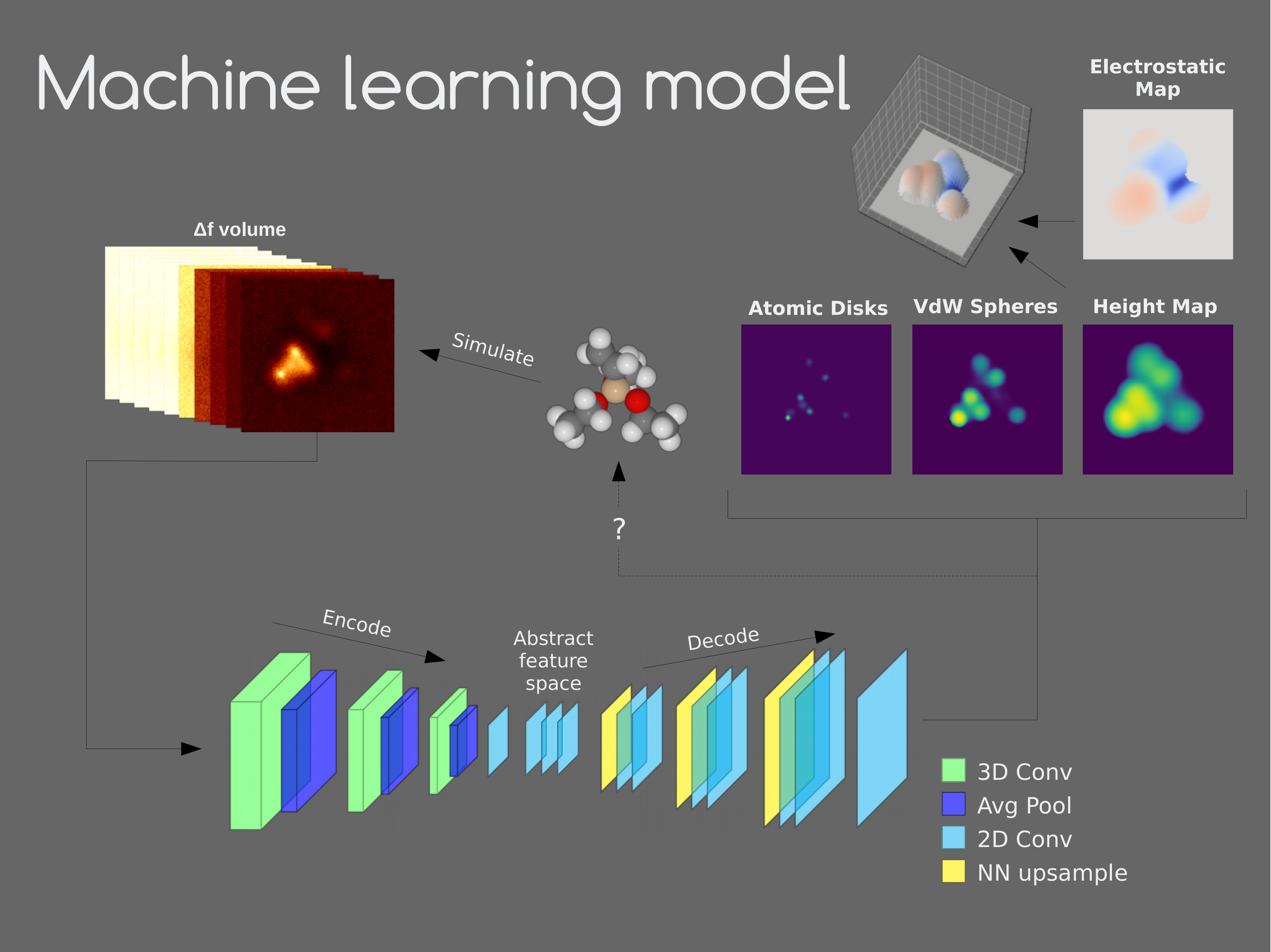
Probe particle relaxation



Probe particle trajectories

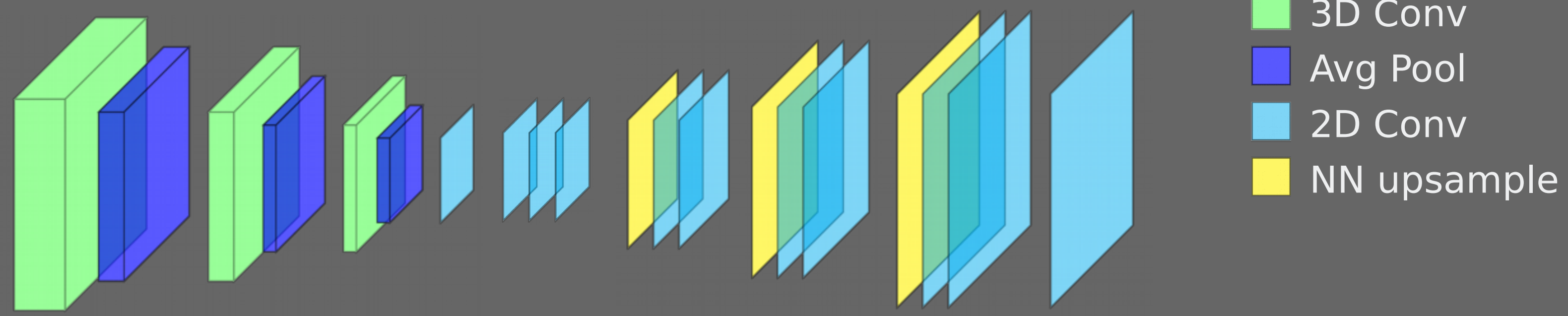
$\Delta\vec{r}$

$\Delta f(\vec{r})$



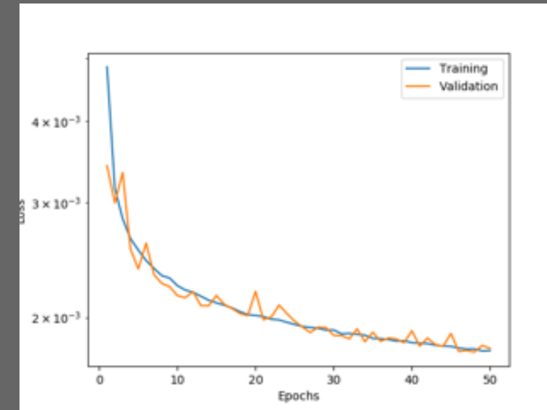
Machine learning model
Electrostatic Map
Δf volume
Simulate
Atomic Disks
VdW Spheres
Height Map
?
Encode
Abstract feature space
Decode
3D Conv
Avg Pool
2D Conv
NN upsample

Model details



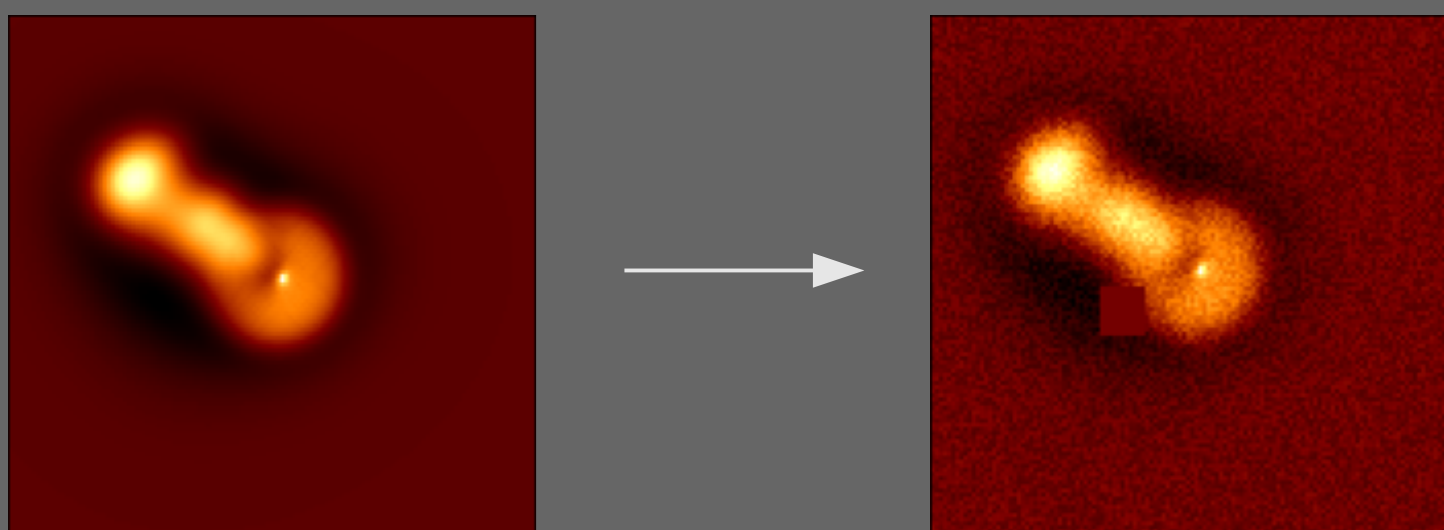
Layer type	Output dimension	Kernel size	Stride	Parameters	Zero padding (x,y,z)
Input	$128 \times 128 \times 10 \times 1$	-	-	-	-
3D conv	$128 \times 128 \times 10 \times 4$	$3 \times 3 \times 3$	$(1,1,1)$	112	$(1,1,1)$
Avg pool	$64 \times 64 \times 5 \times 4$	$2 \times 2 \times 2$	$(2,2,2)$	-	-
3D conv	$64 \times 64 \times 5 \times 8$	$3 \times 3 \times 3$	$(1,1,1)$	872	$(1,1,1)$
Avg pool	$32 \times 32 \times 2 \times 8$	$2 \times 2 \times 2$	$(2,2,2)$	-	-
3D conv	$32 \times 32 \times 2 \times 16$	$3 \times 3 \times 3$	$(1,1,1)$	3472	$(1,1,1)$
Avg pool	$16 \times 16 \times 2 \times 16$	$2 \times 2 \times 1$	$(2,2,1)$	-	-
Parallel 2D convs	$16 \times 16 \times 128$	3×3	$(1,1)$	5888	$(1,1)$
2D conv	$16 \times 16 \times 64$	1×1	$(1,1)$	8256	$(1,1)$
2D conv	$16 \times 16 \times 64$	3×3	$(1,1)$	36928	$(1,1)$
2D conv	$16 \times 16 \times 64$	3×3	$(1,1)$	36928	$(1,1)$
NN-upsample	$32 \times 32 \times 64$	-	-	-	-
2D conv	$32 \times 32 \times 16$	3×3	$(1,1)$	9232	$(1,1)$
2D conv	$32 \times 32 \times 16$	3×3	$(1,1)$	2320	$(1,1)$
NN-upsample	$64 \times 64 \times 16$	-	-	-	-
2D conv	$64 \times 64 \times 16$	3×3	$(1,1)$	2320	$(1,1)$
2D conv	$64 \times 64 \times 16$	3×3	$(1,1)$	2320	$(1,1)$
NN-upsample	$128 \times 128 \times 16$	-	-	-	-
2D conv	$128 \times 128 \times 16$	3×3	$(1,1)$	2320	$(1,1)$
2D conv	$128 \times 128 \times 16$	3×3	$(1,1)$	2320	$(1,1)$
2D conv	$128 \times 128 \times 1$	3×3	$(1,1)$	145	$(1,1)$

Model training



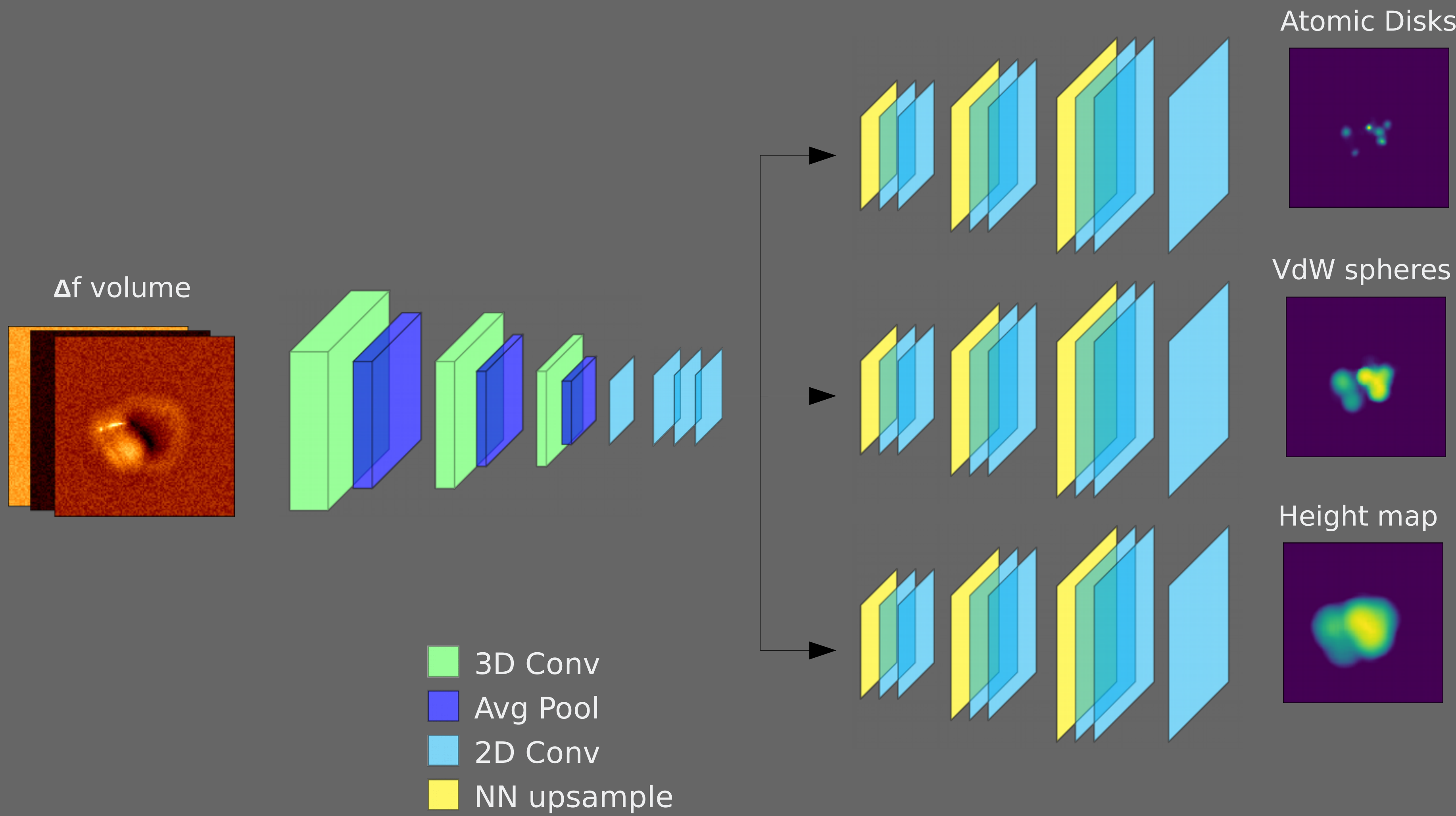
- Keras + Tensorflow
- Mean squared loss $\frac{1}{N_{pixels}} \sum_{i=1}^{N_{pixels}} (f(x)_i - y_i)^2$
- Trained on 5000-6000 molecules with 20 rotations each

  → ~100000 training samples
- Regularization: Random noise, Cutouts, Random pixel shift, Scanning height randomization



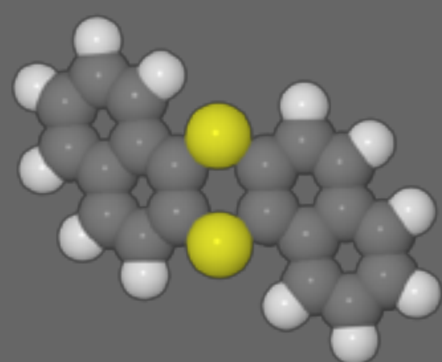
Results

Positional prediction

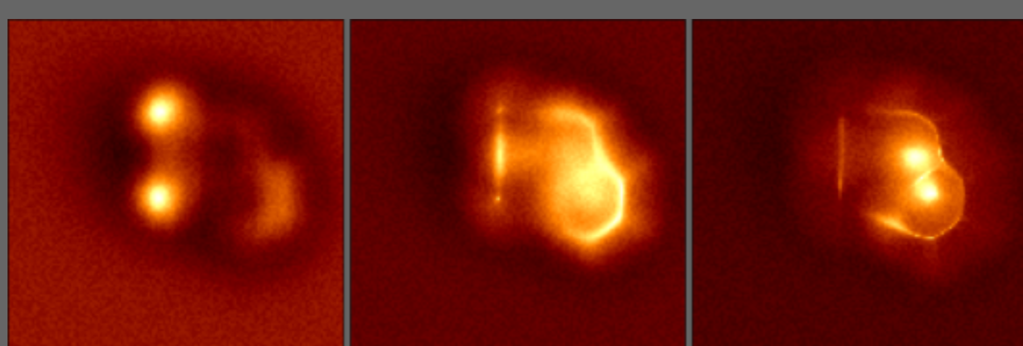


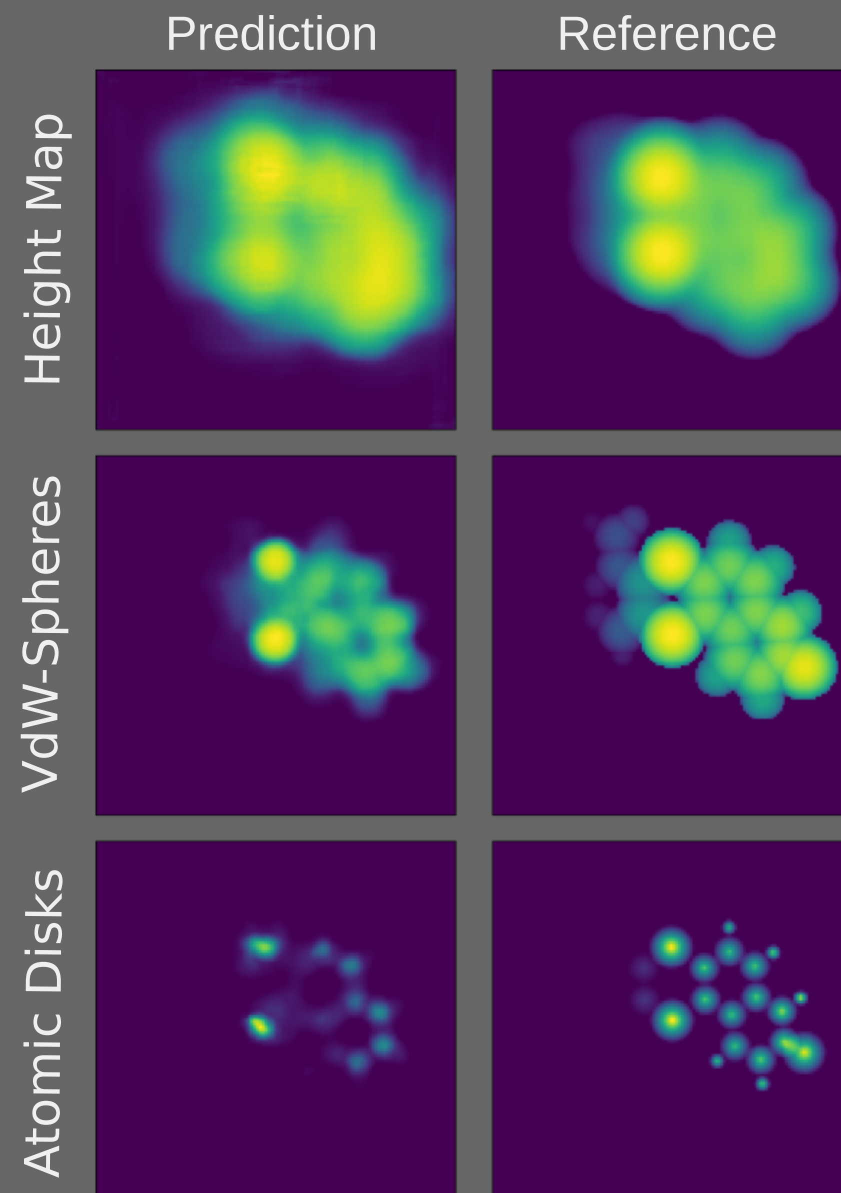
Simulations

Dibenzo[a,h]-thianthrene

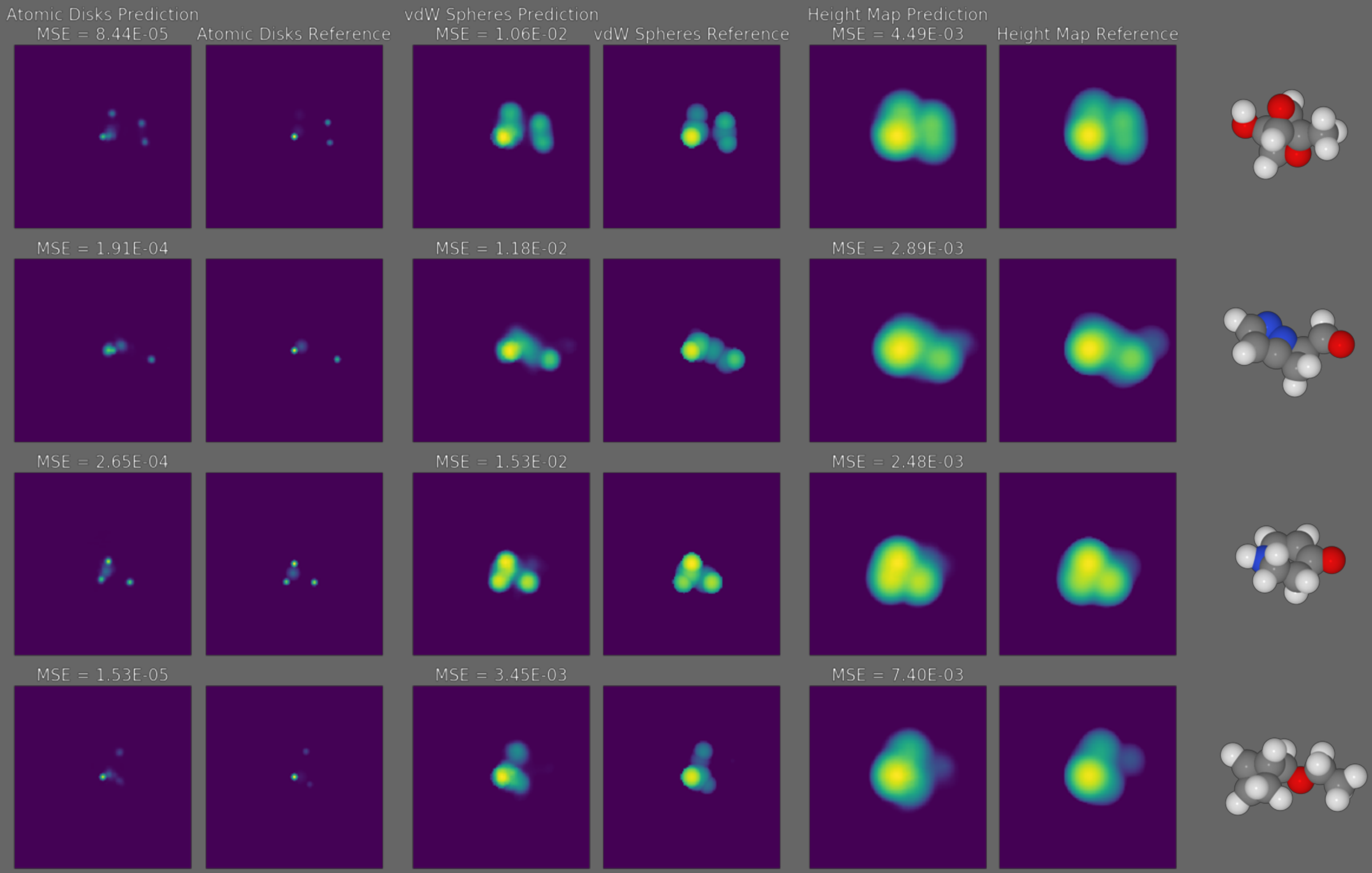


Simulated Δf

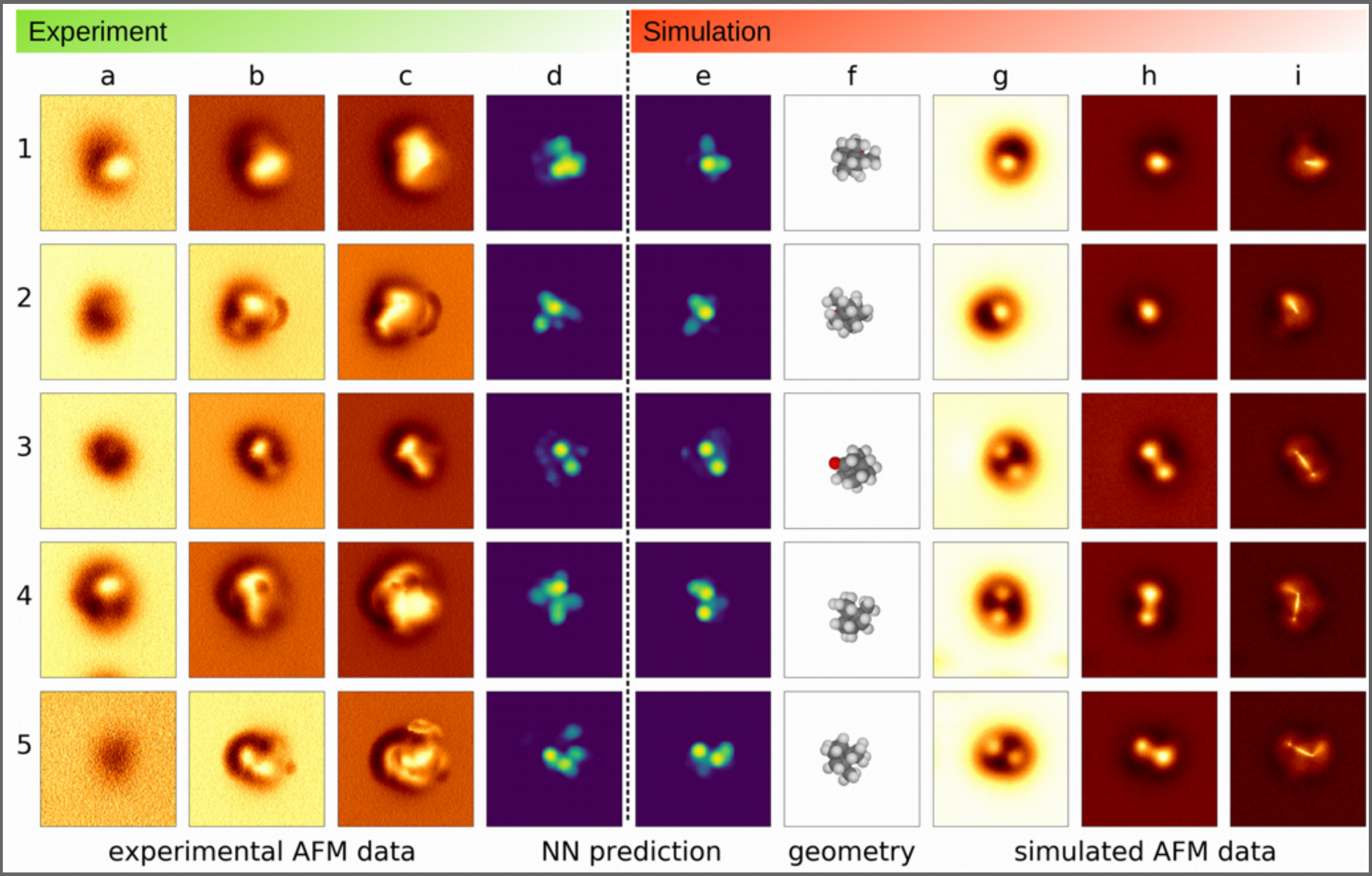




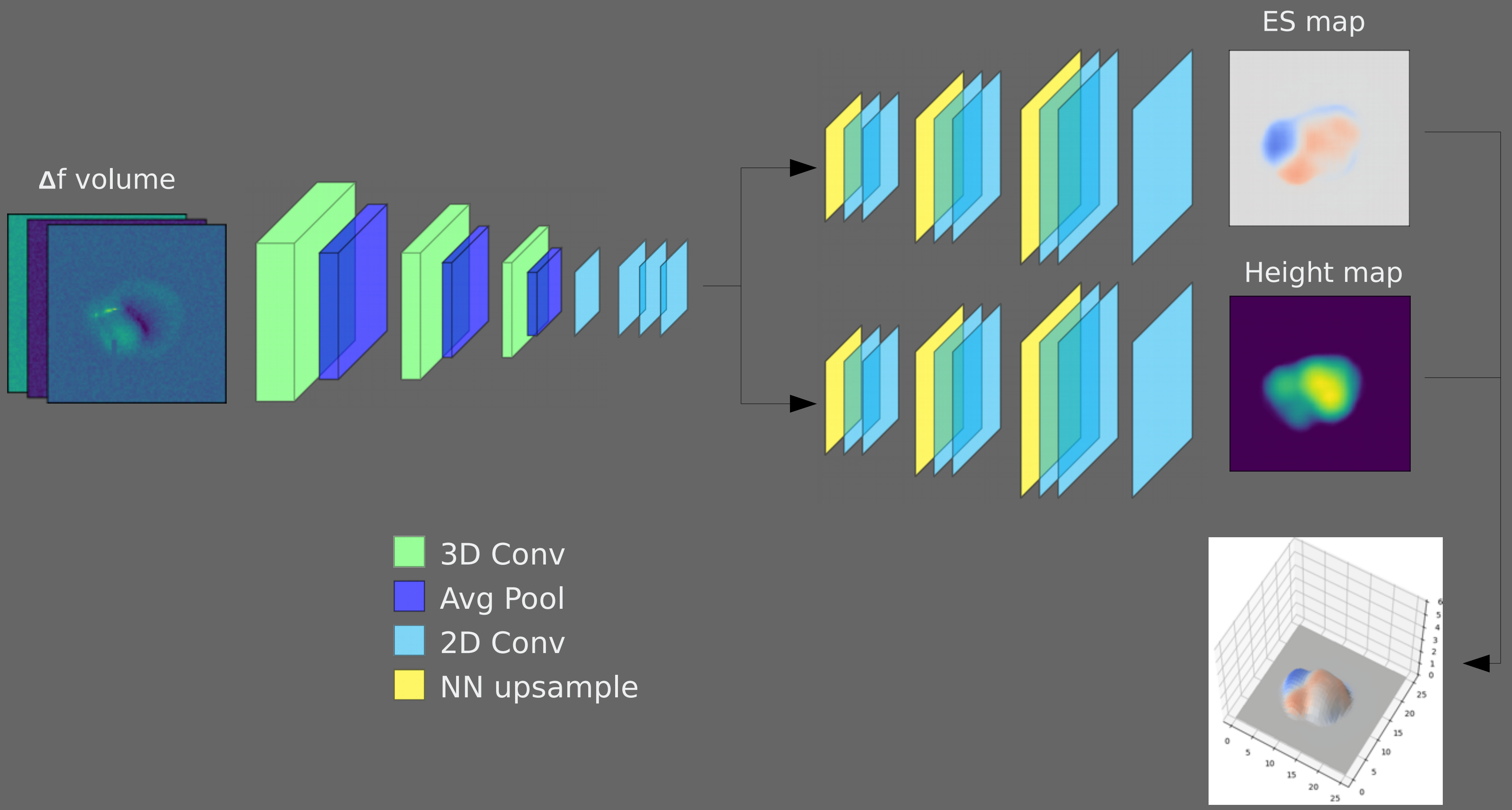
Few more examples



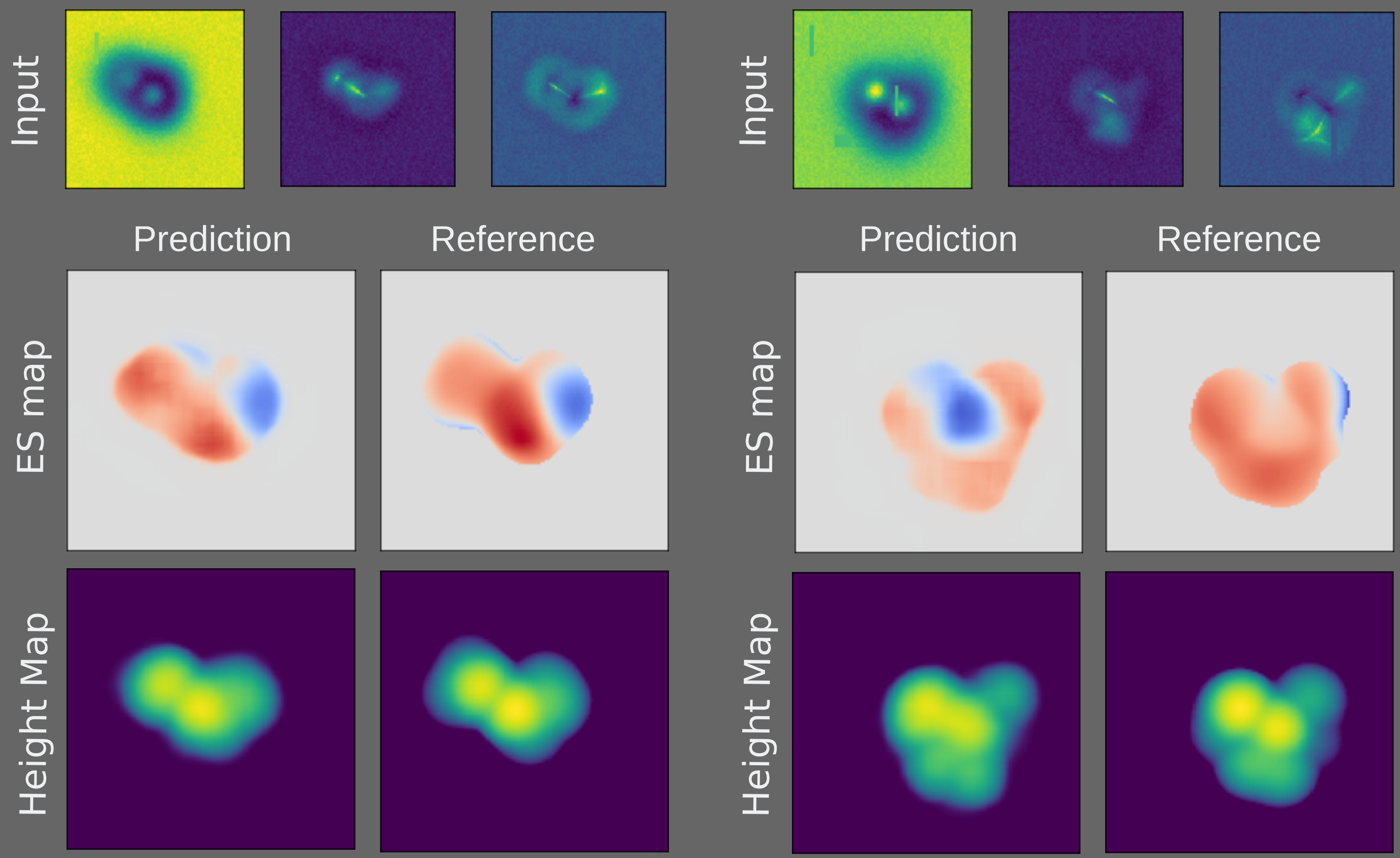
Experimental



Electrostatics prediction

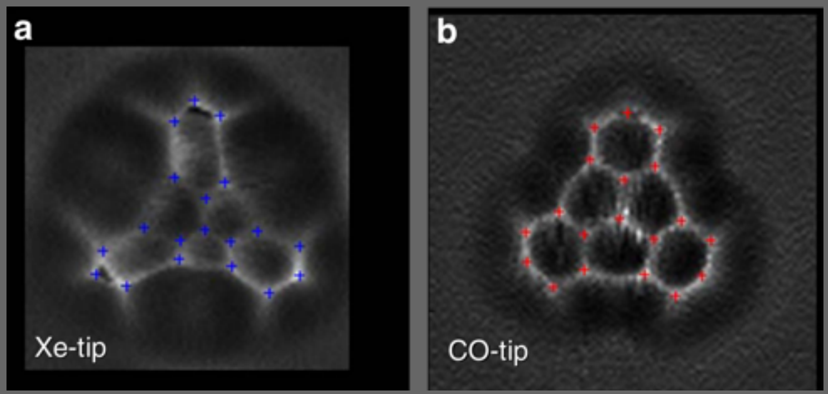


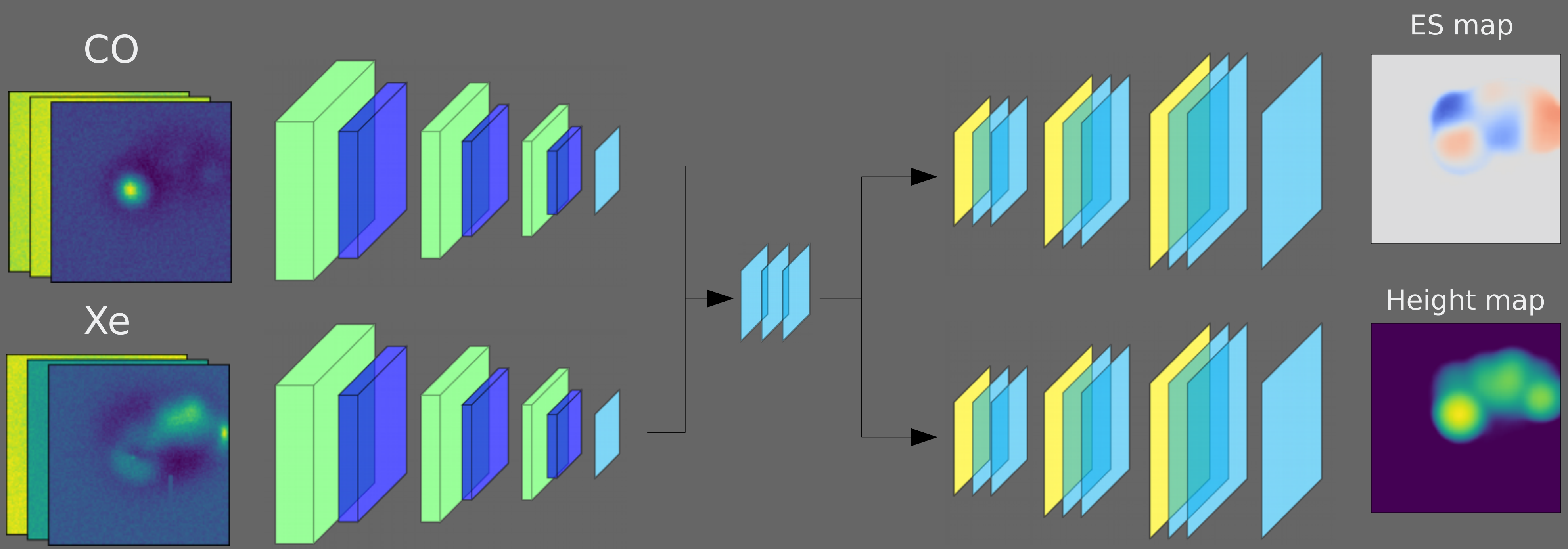
Electrostatics prediction



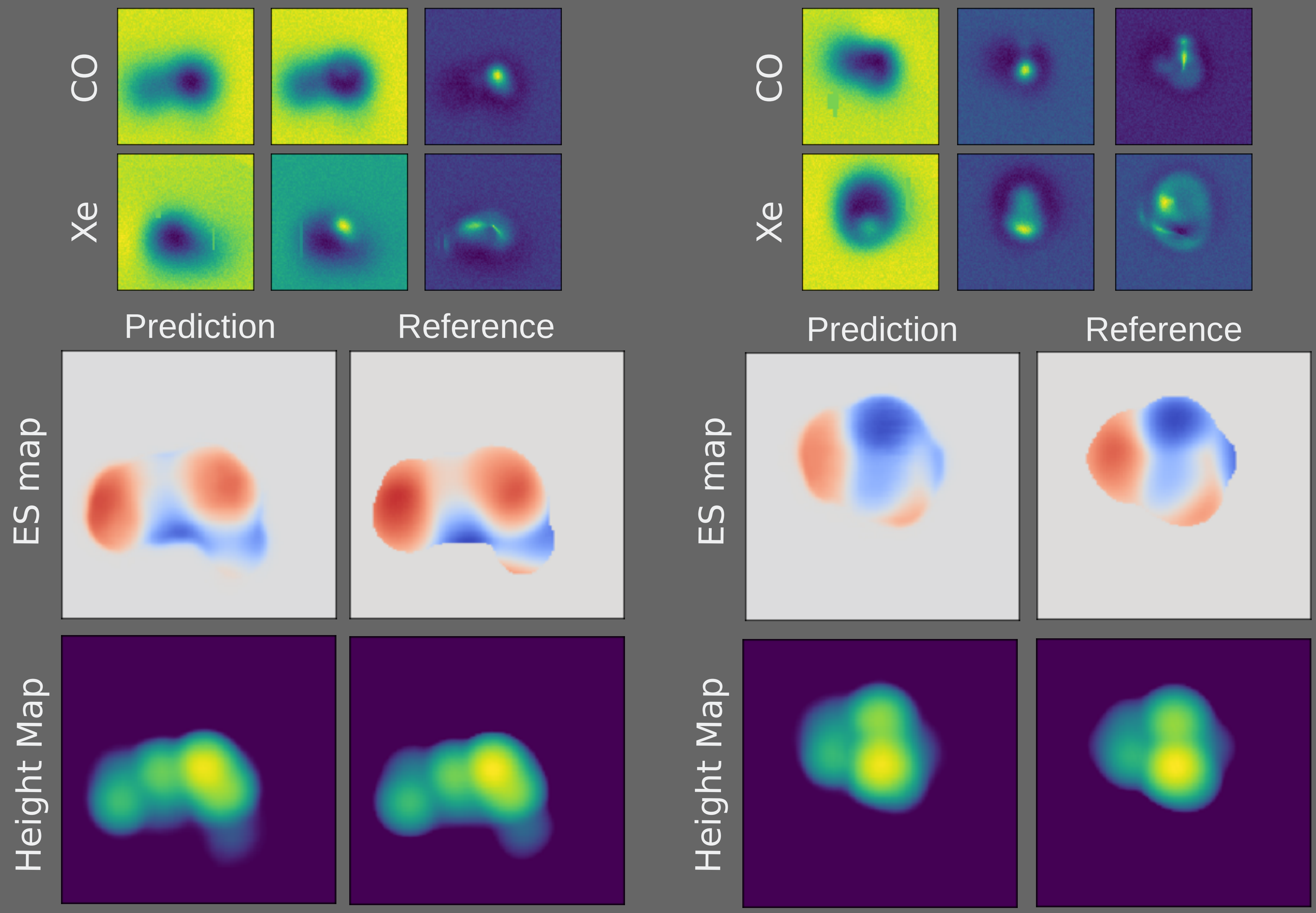
Multiple inputs

Hapala et al. (2016)



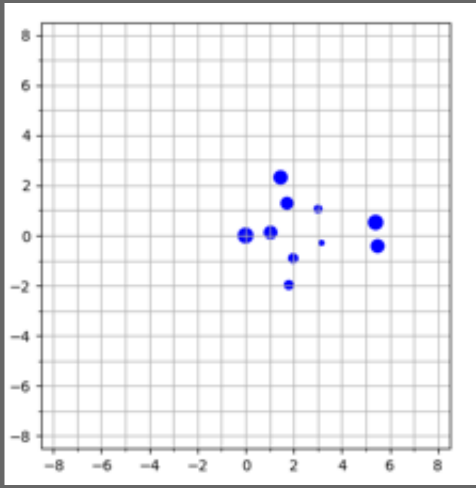


Multi-input electrostatics



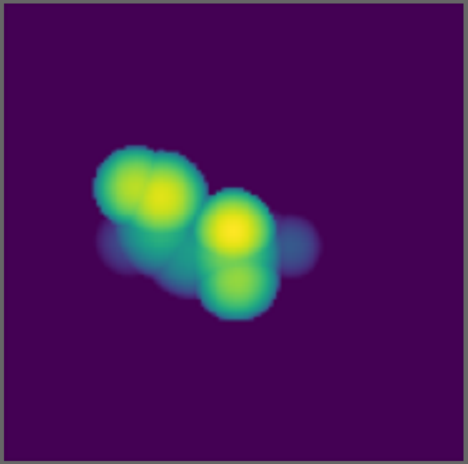
Future directions

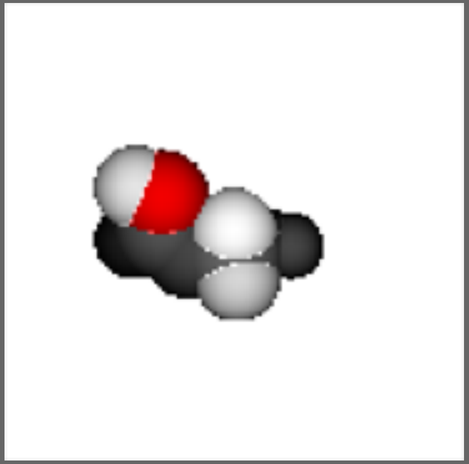
Direct prediction of coordinates



(9.80, 6.02, -0.61),
(9.98, 7.08, -0.58),
(9.03, 8.11, -0.26),
(11.16, 7.70, -0.84),
...

Predicting elements





In conclusion

- ML model for predicting properties from AFM images
- Good performance on simulated images
- Experimental images remain challenging