Remote and on-the-fly: artificial intelligence driven science in laboratories and central facilities.

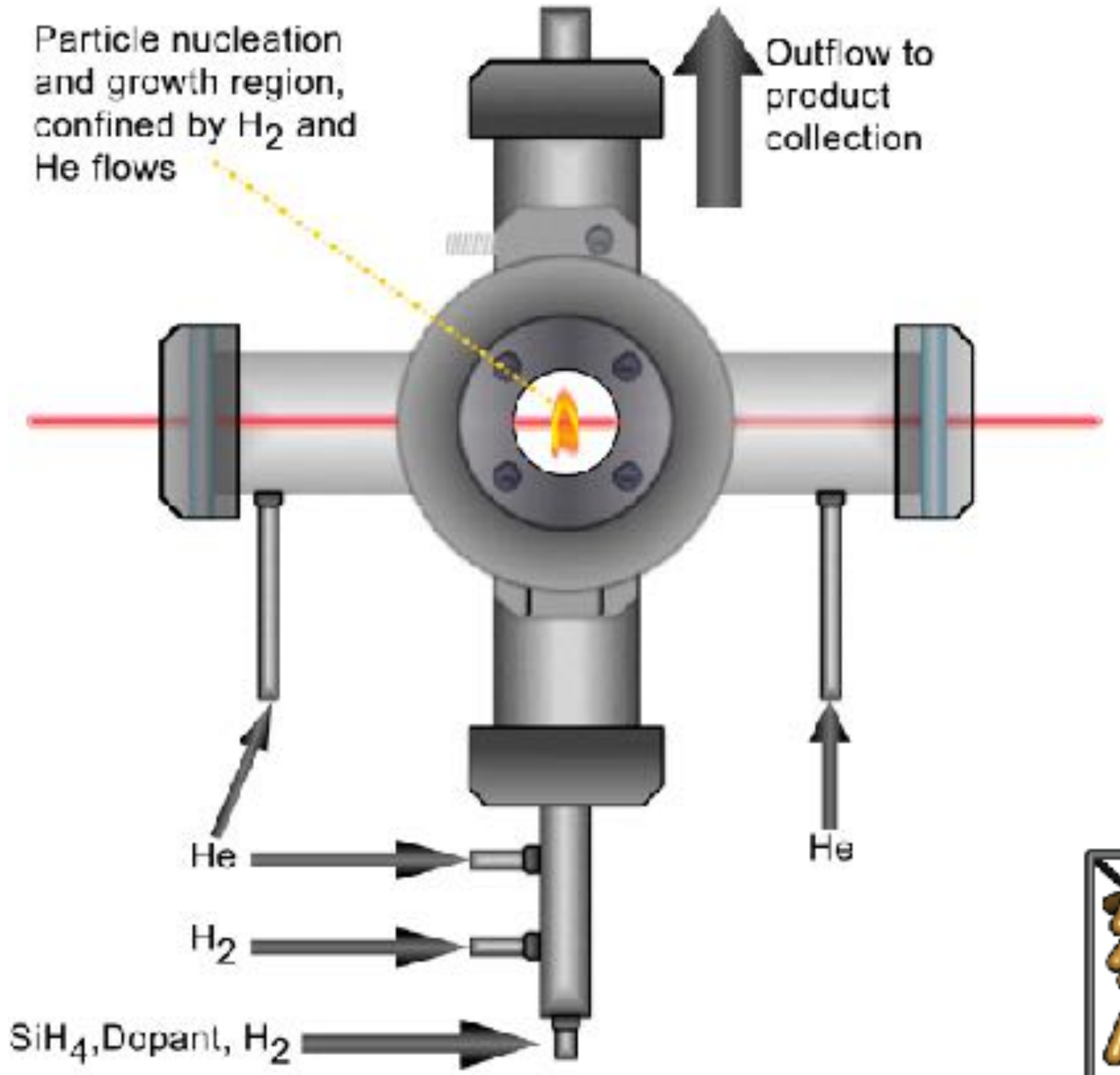
Dr. Phil Maffettone

NYSDS Oct 2021

U.S. DEPARTMENT OF ENERGY | Office of Science

BROOKHAVEN NATIONAL LABORATORY

maffettone@dssi:~/$ whoami



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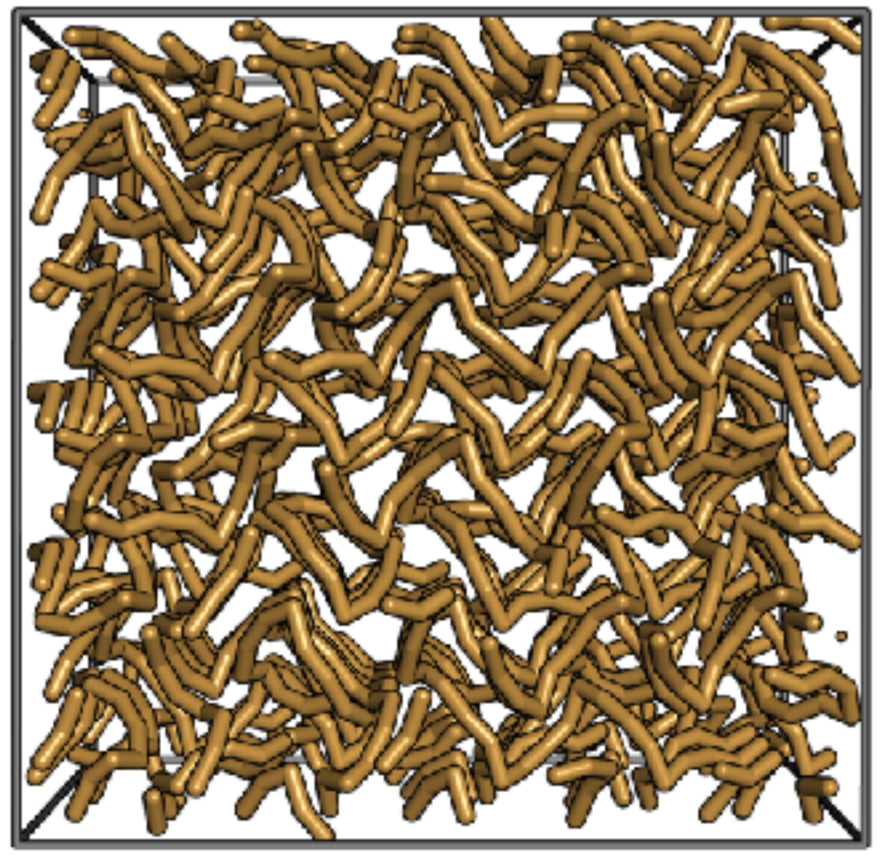

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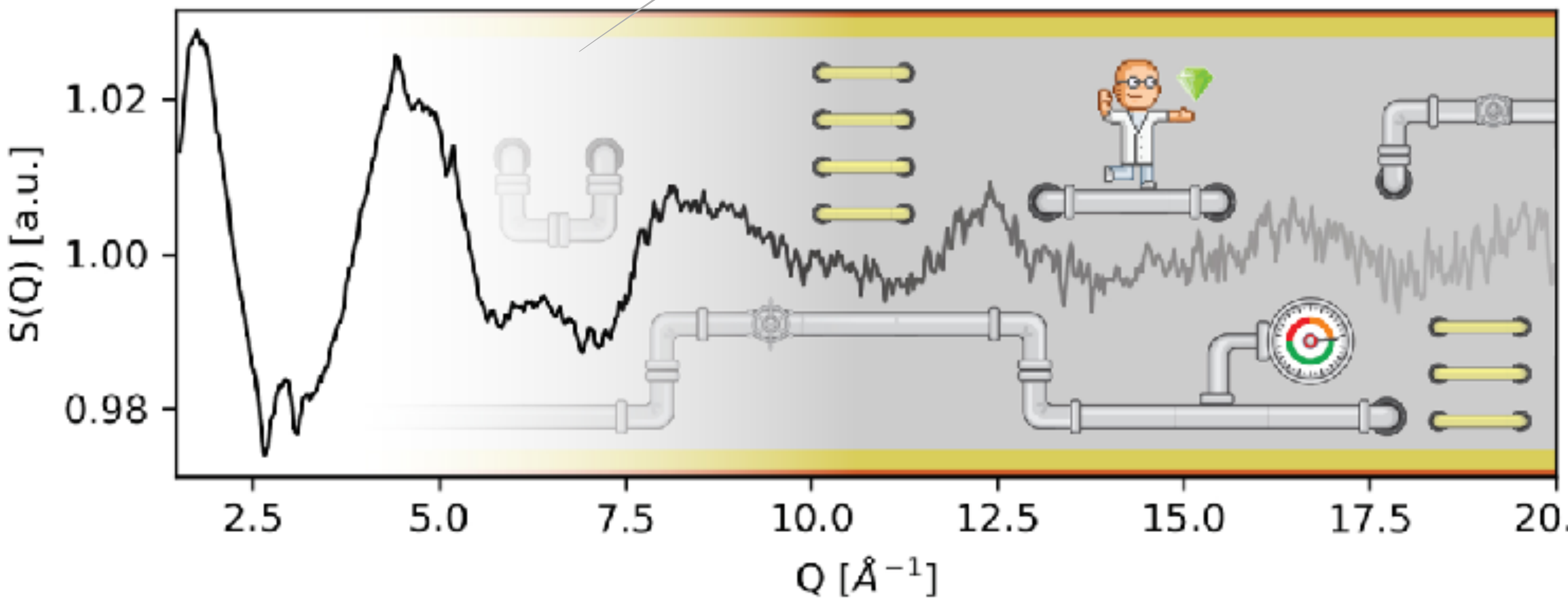

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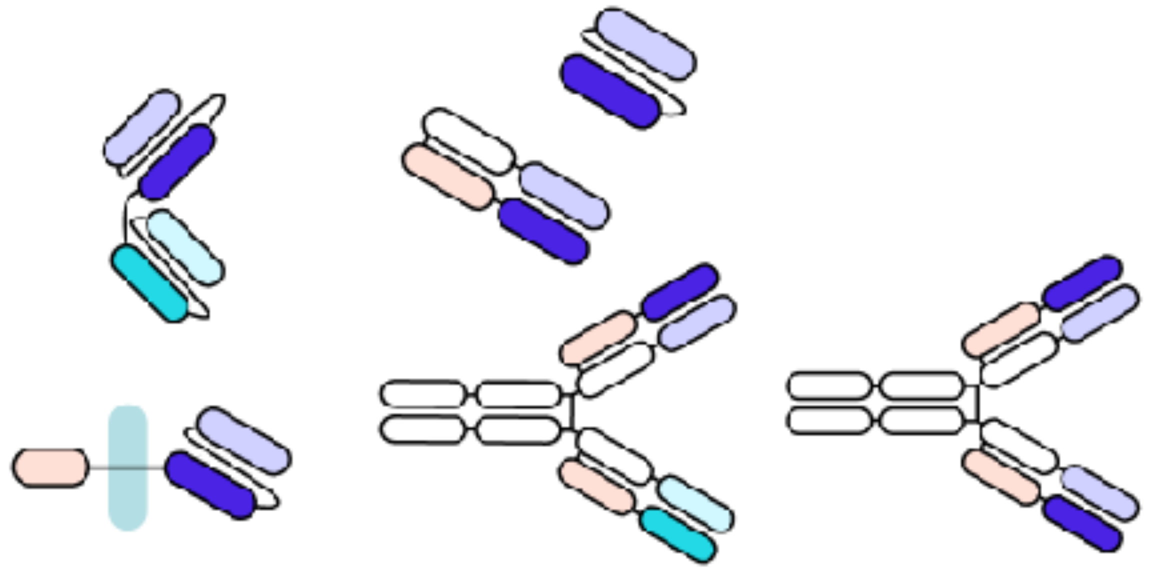

maffettone@dssi:~/$ members {ALL}

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BigHat Biosciences

Dr. Peyton Greenside

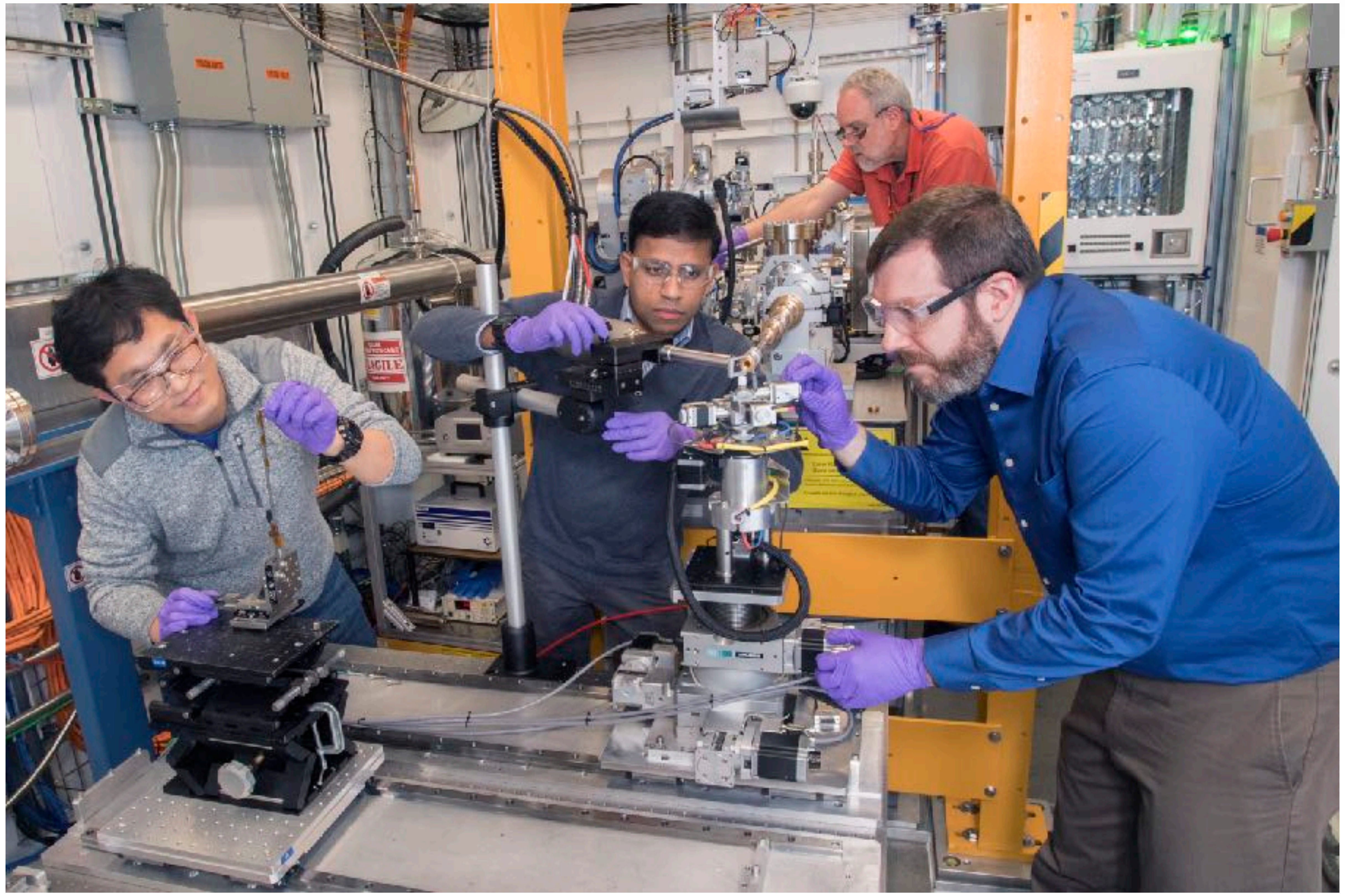
Dr. Emily Delany

Vivek Myers

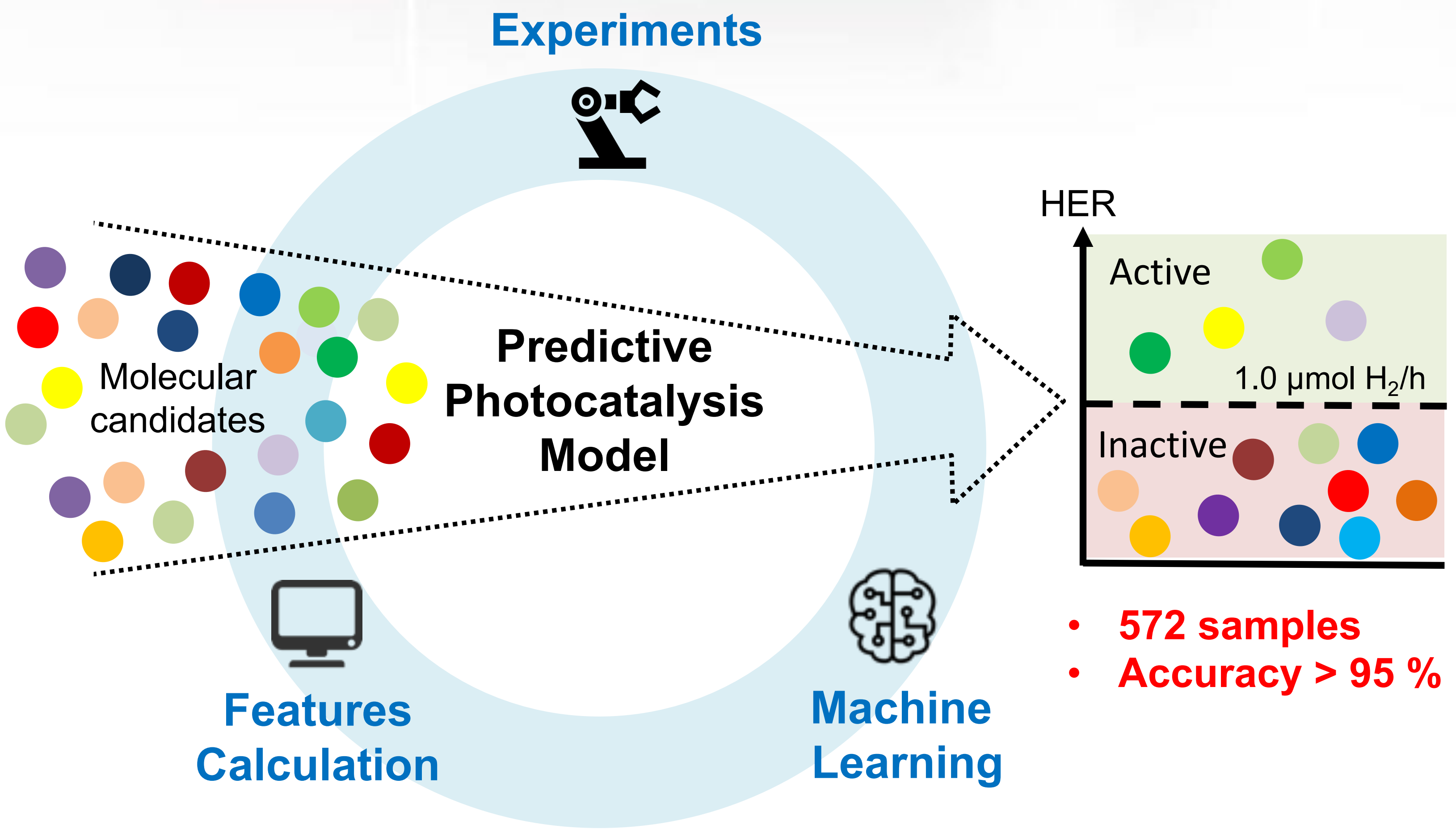
Aaron Solomon

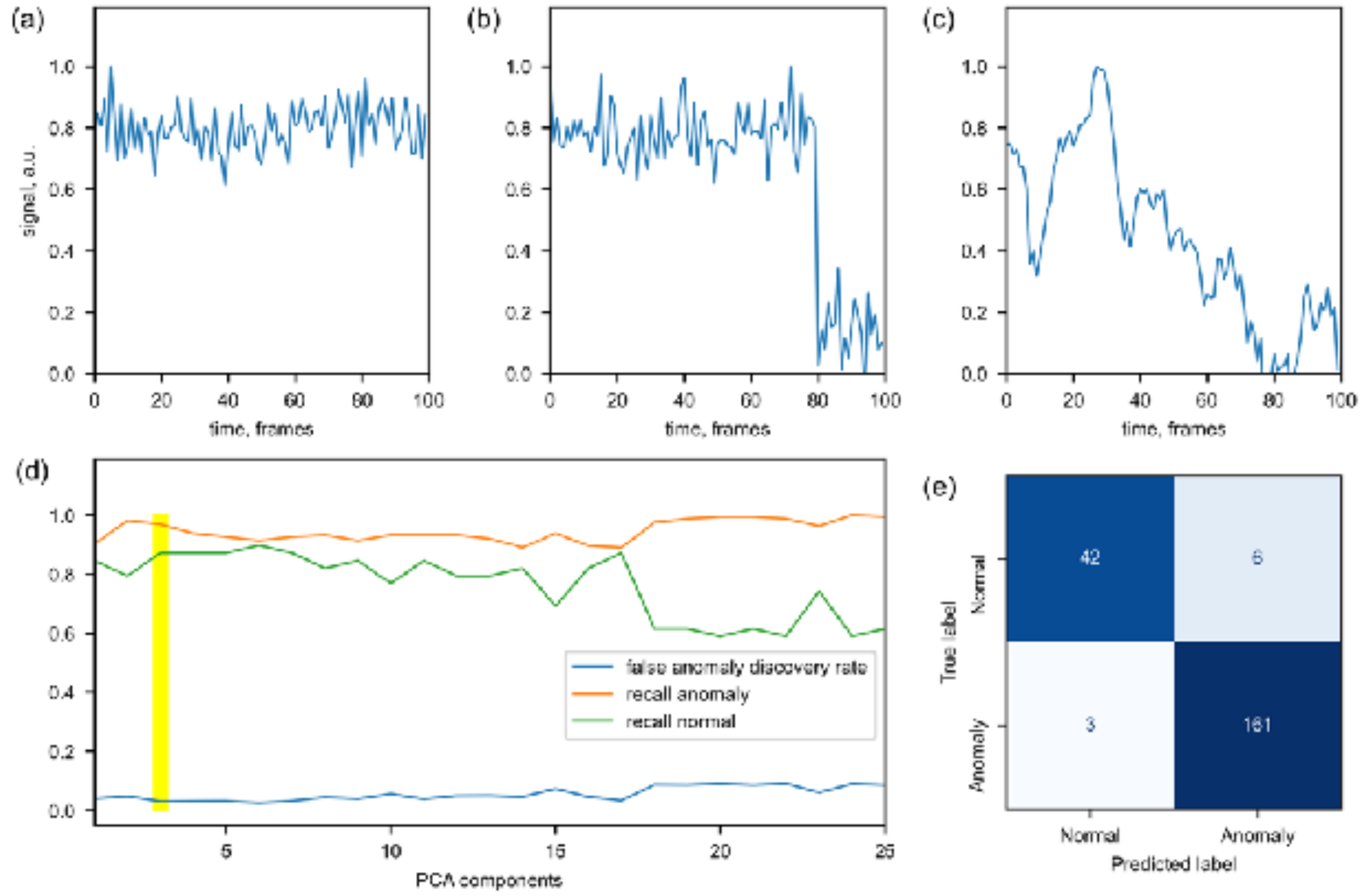
Federated AI, data streaming, and pragmatic engineering

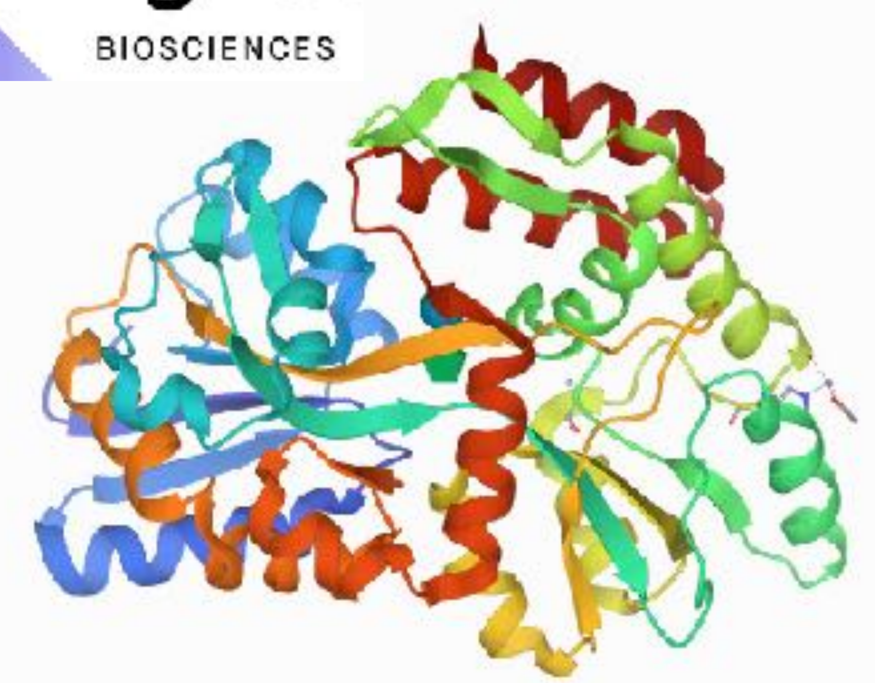
- There is no one-size-fits-all AI/ML approach for any science.
- Federations of agents can solve different tasks asynchronously.
- Data streaming enables this.
- Collaboration drawing on domain knowledge and AI/ML expertise results in the most impactful projects.

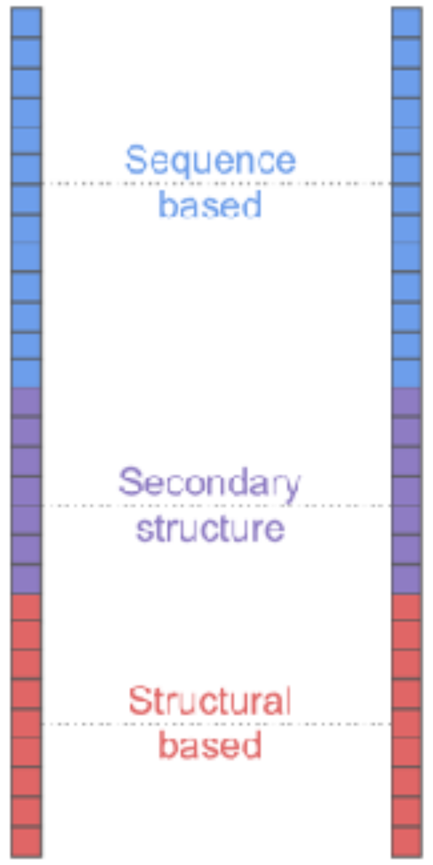


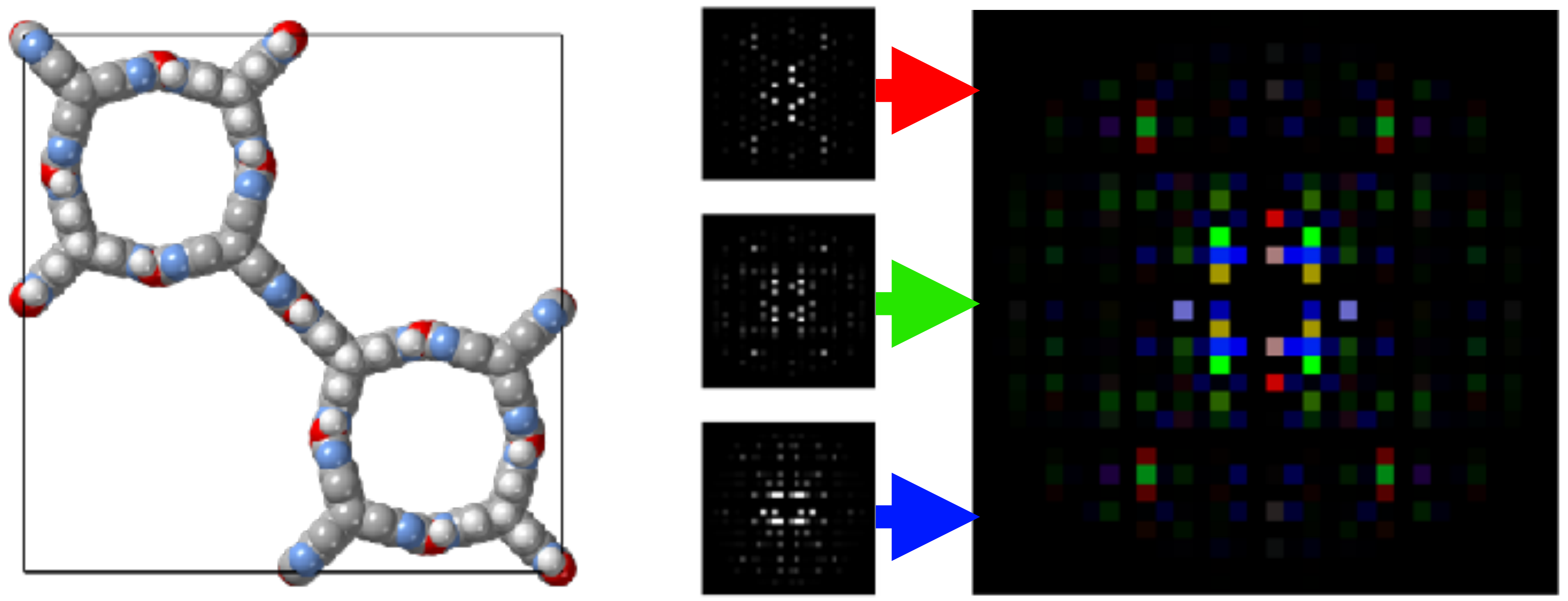
Feature engineering can be incredibly effective, and requires collaboration with domain experts.







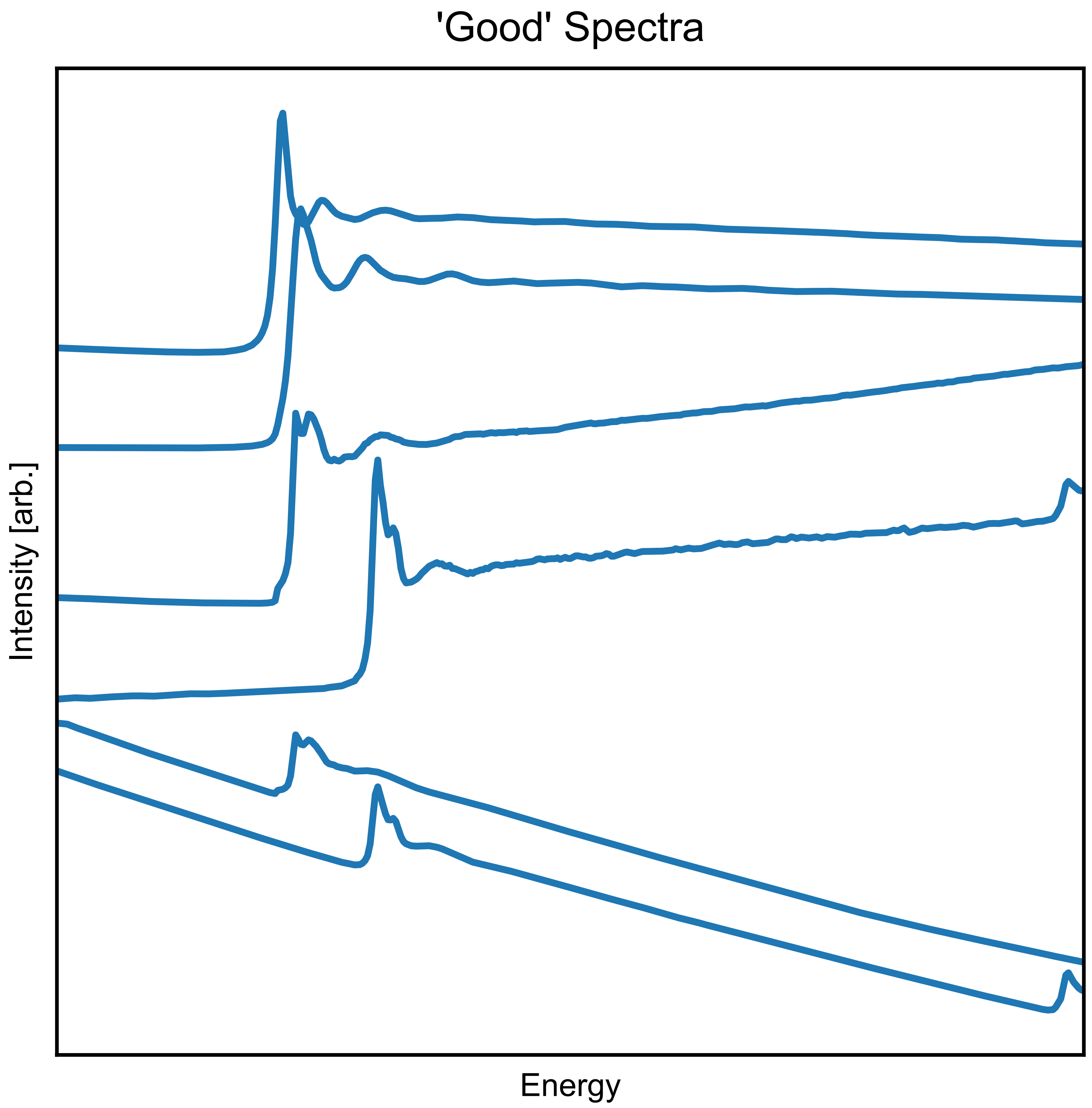


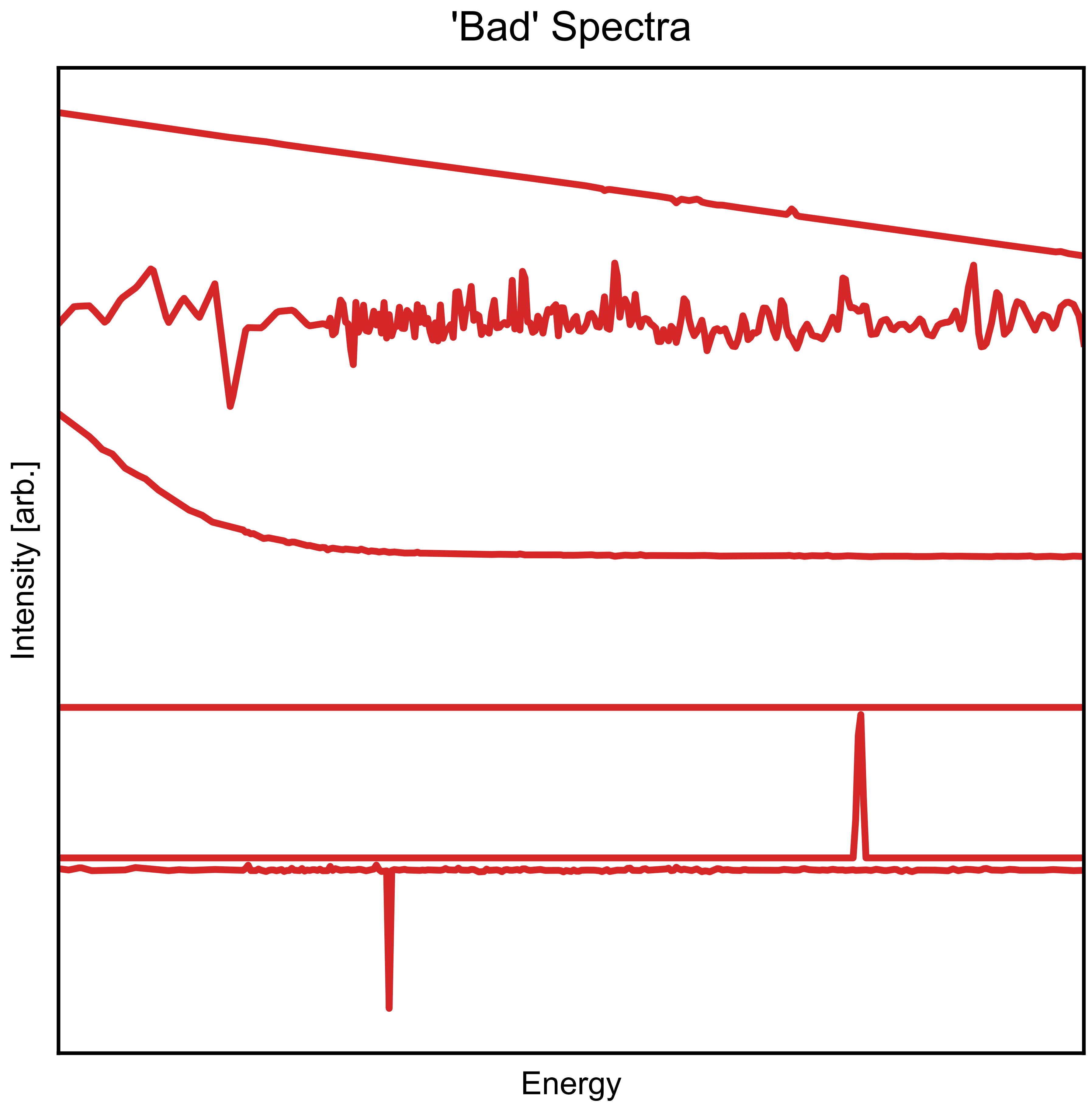


Supervised learning:

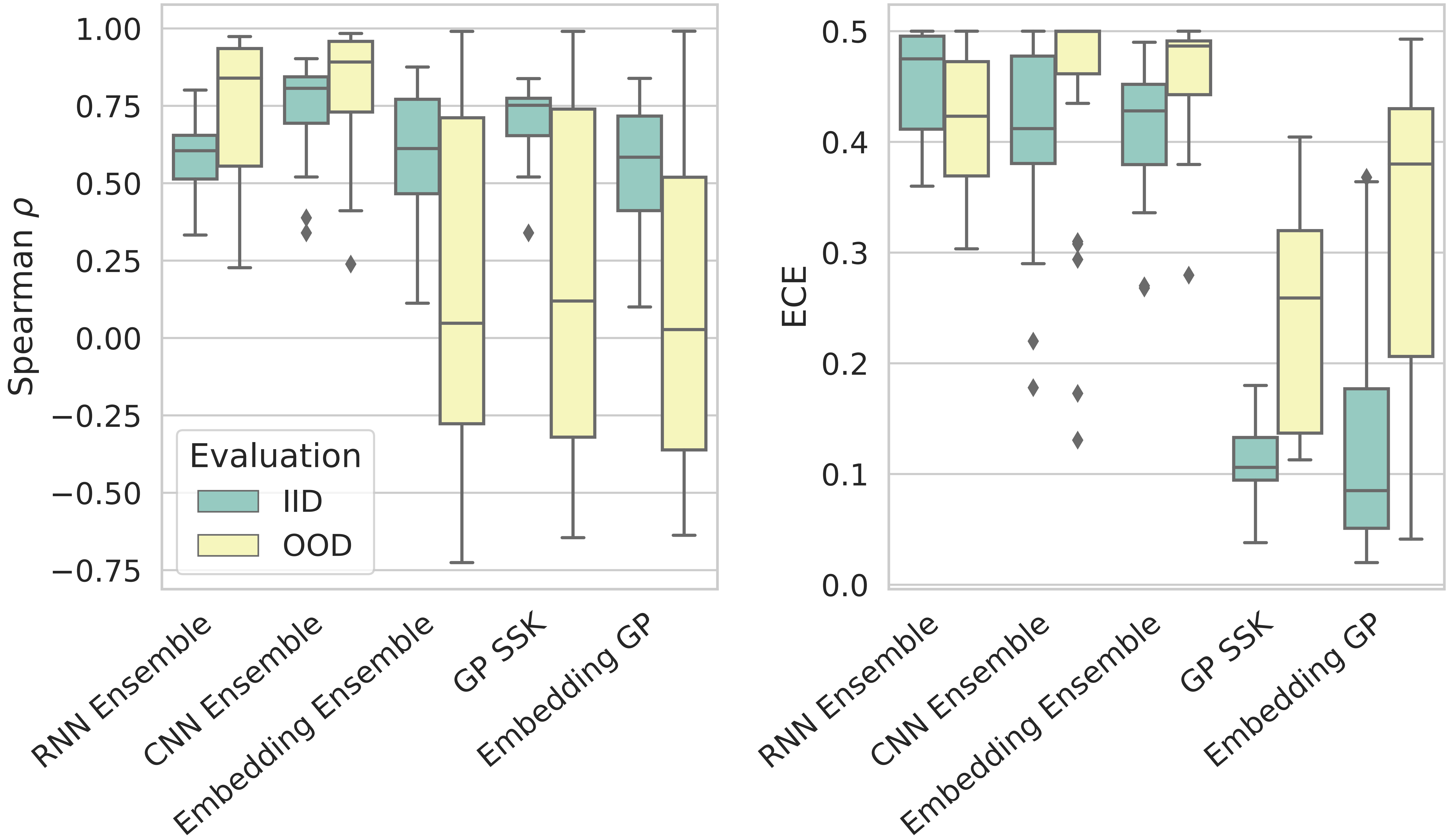
Predicting labels for data when we have–or can create–labeled datasets.

Identifying experimental failures at BMM.



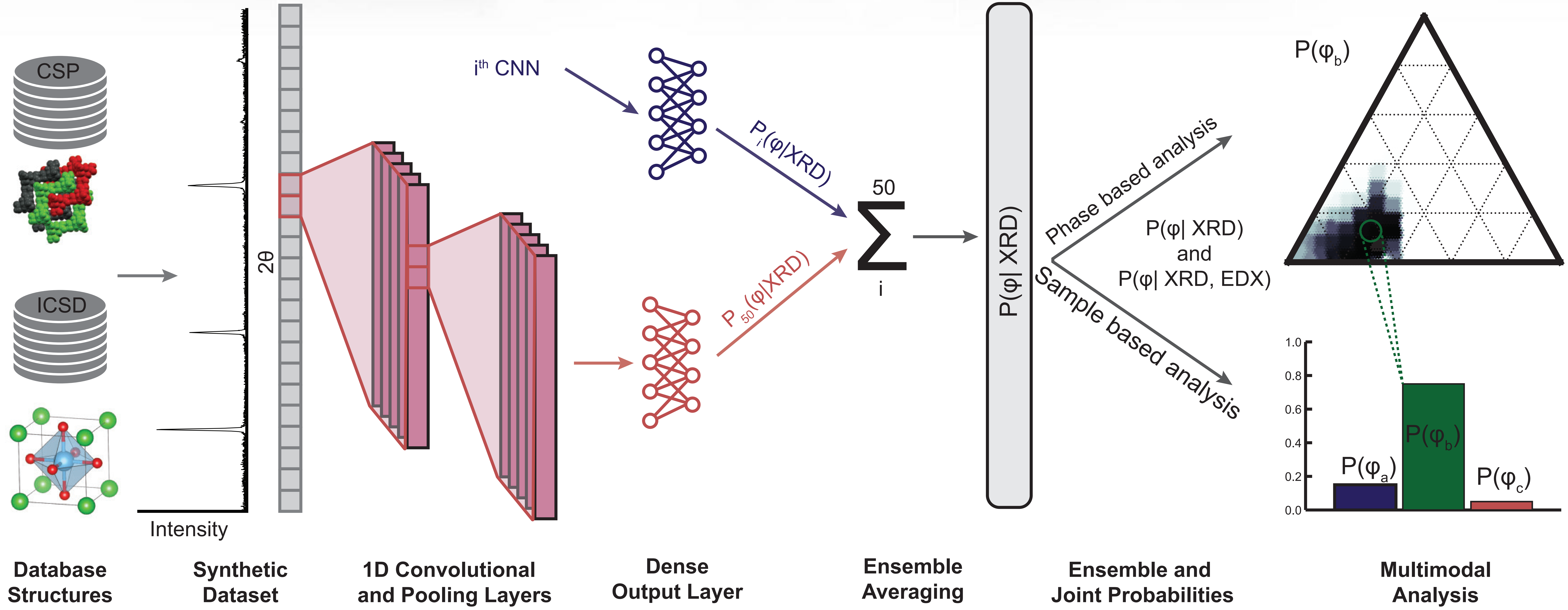


Testing a suite of algorithms and featurizations for describing the functional response of a fluorescent protein.



Gruver, N. *et al., ICML 2020*

A fully synthetic data pipeline can train an accurate probabilistic model prior to the experiment.



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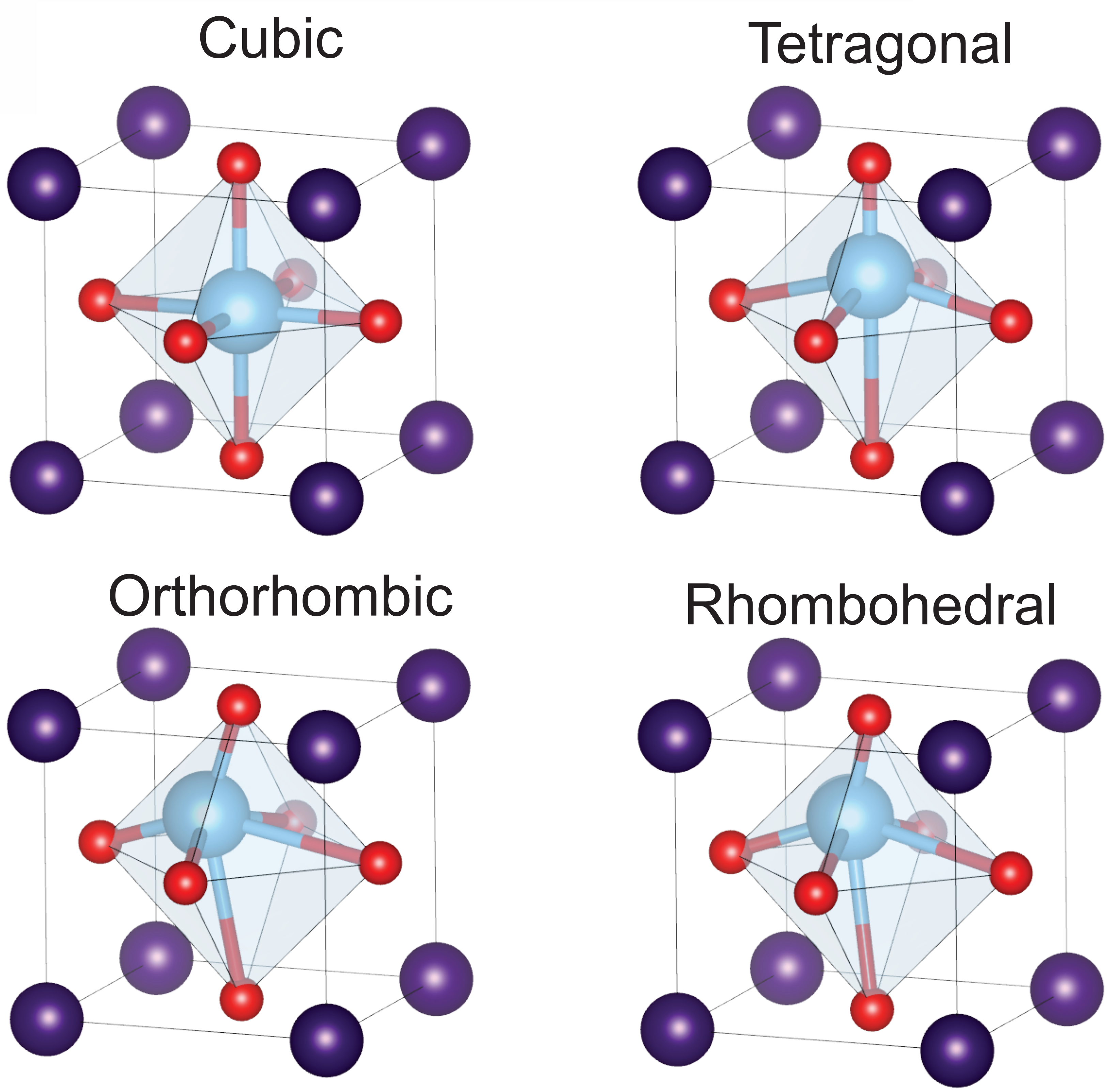
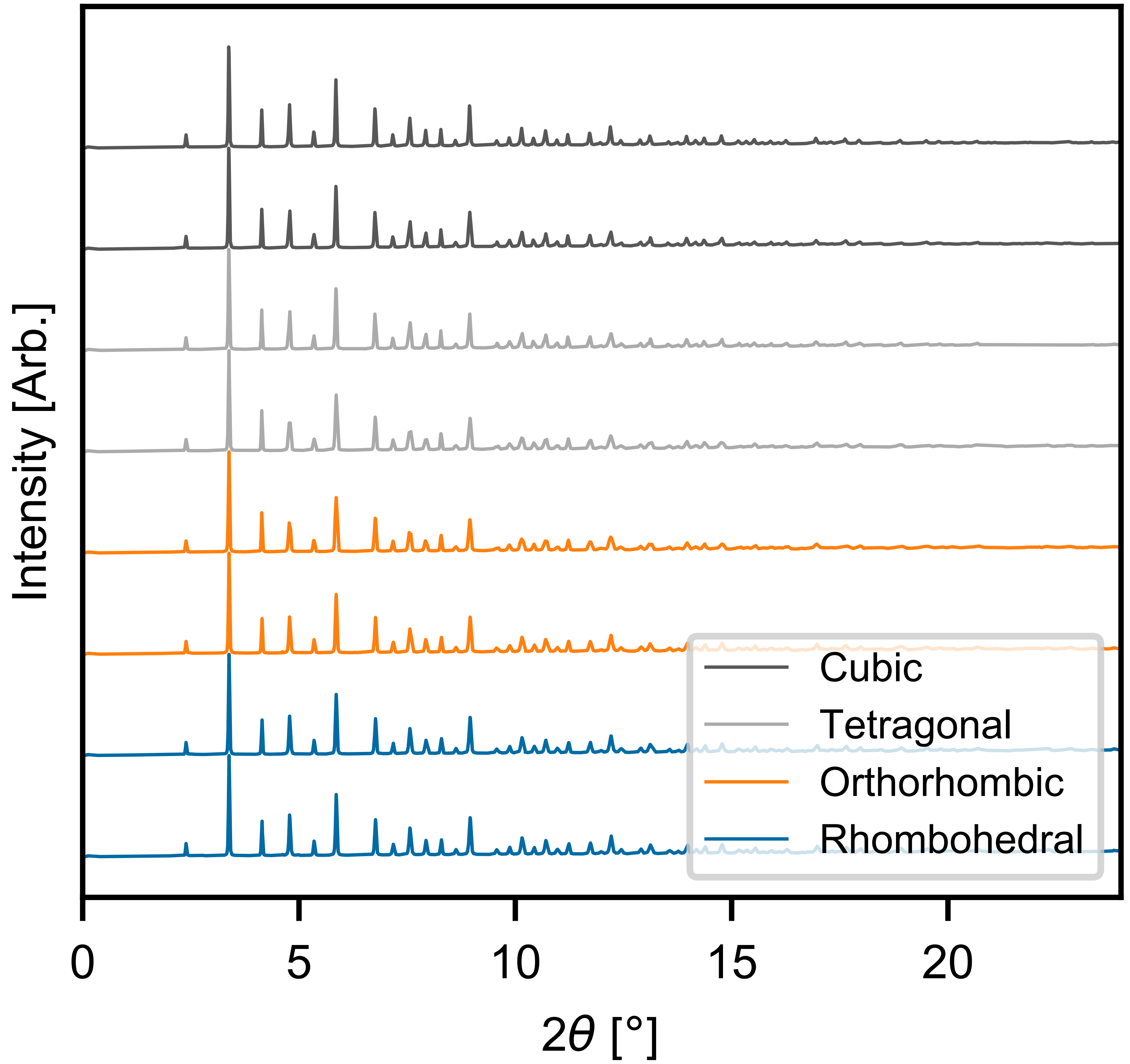
Maffettone, P.M. *et al.*, *Nat. Comp. Sci.*, **1**, 290-297 (2021)

Classifying subtle phase transitions in $BaTiO_3$.





Maffettone, P.M. *et al.*, *Nat. Comp. Sci.*, **1**, 290-297 (2021)

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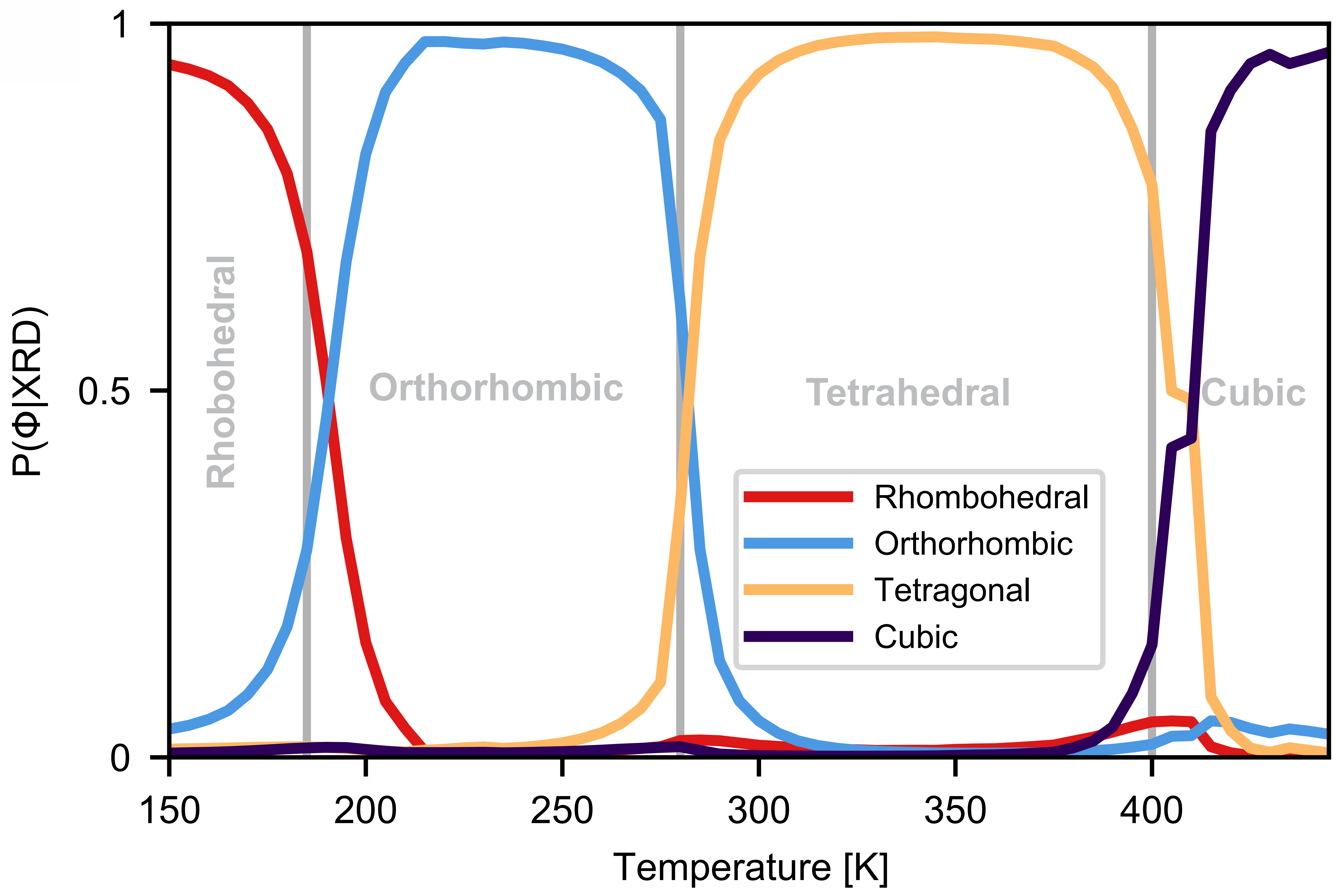
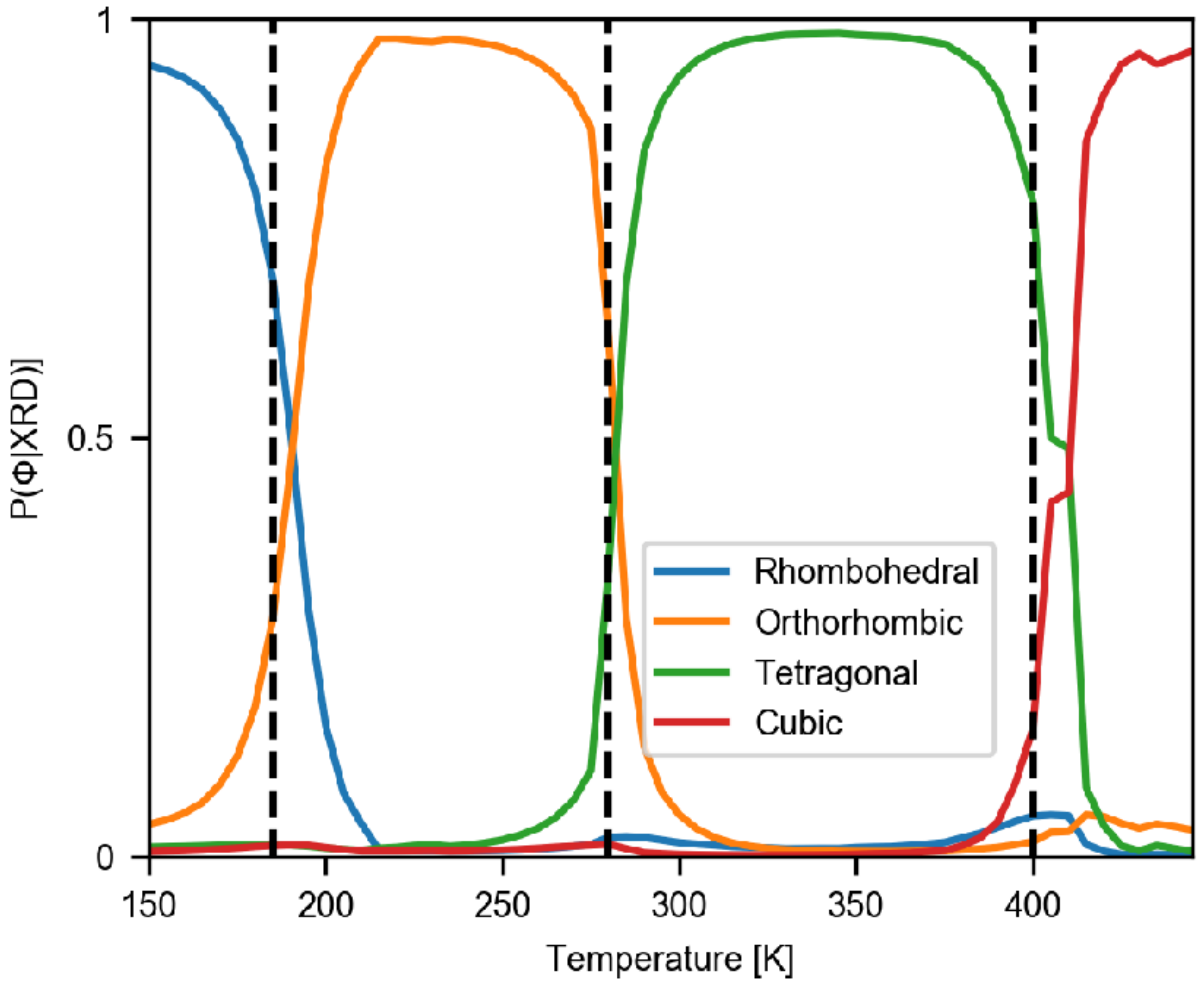


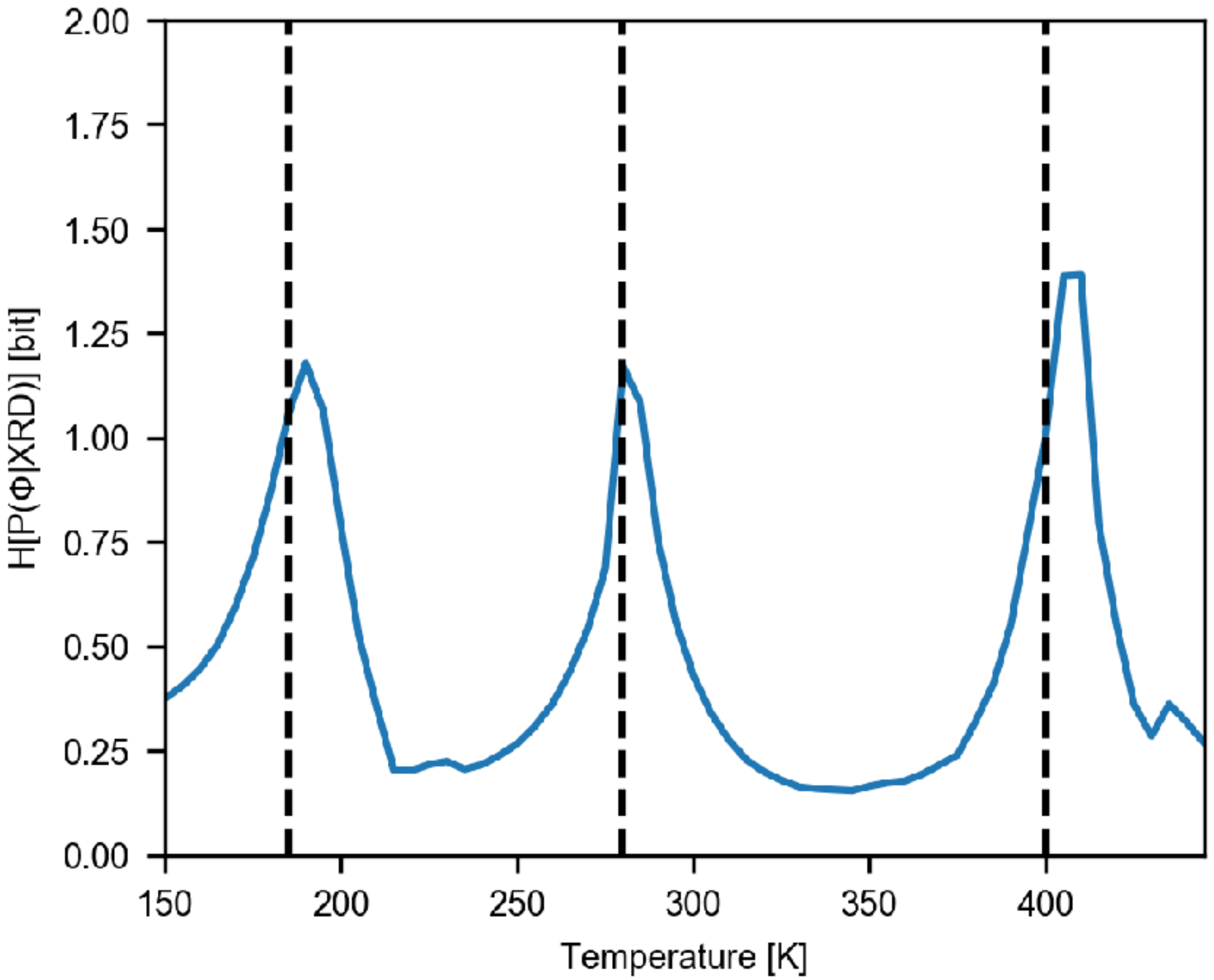
Maffettone, P.M. *et al.*, *Nat. Comp. Sci.*, **1**, 290-297 (2021)

Unsupervised learning:

How do we approach situations when we are exploring the unknown?

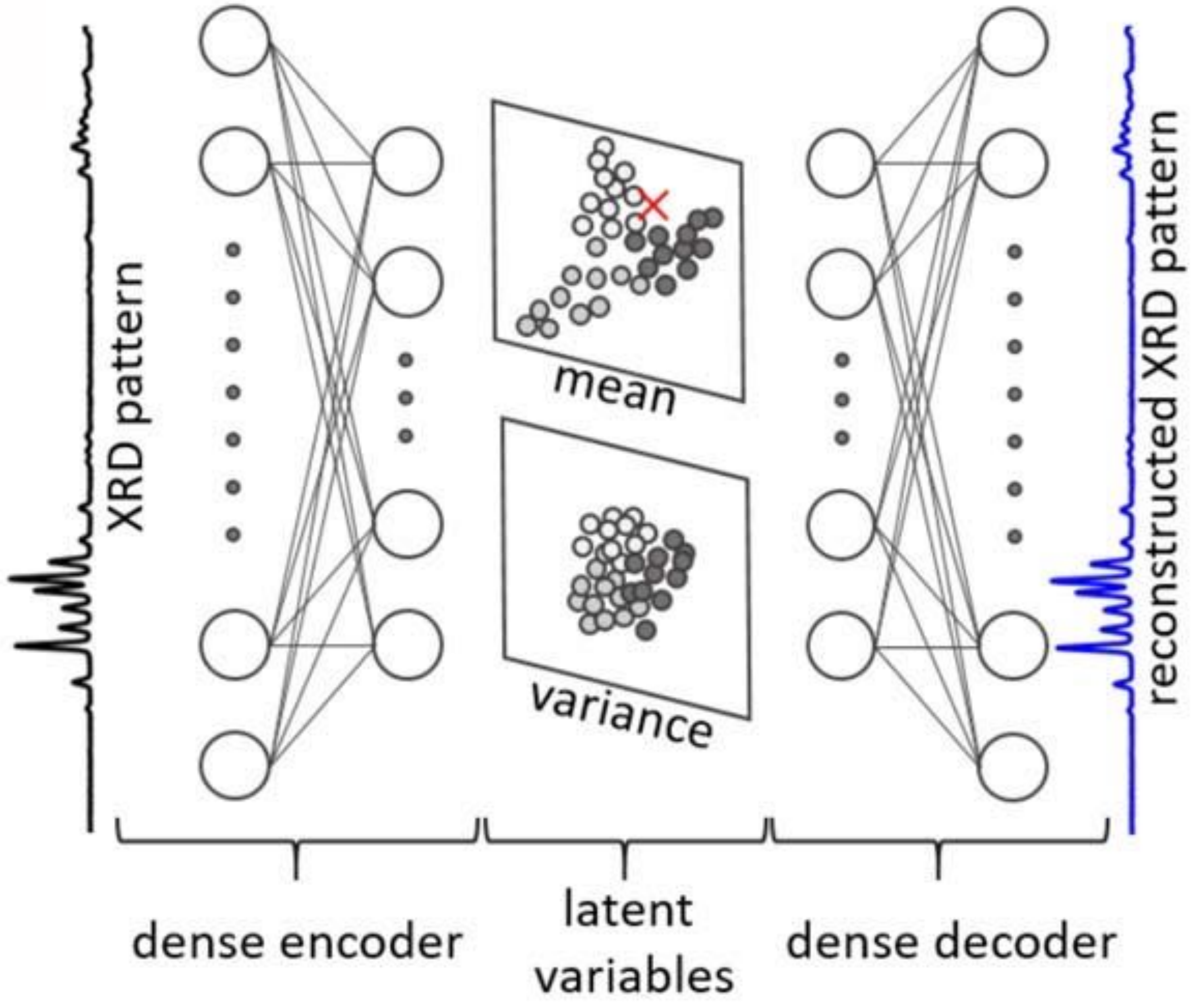
Uncertainty is a proxy for novelty.

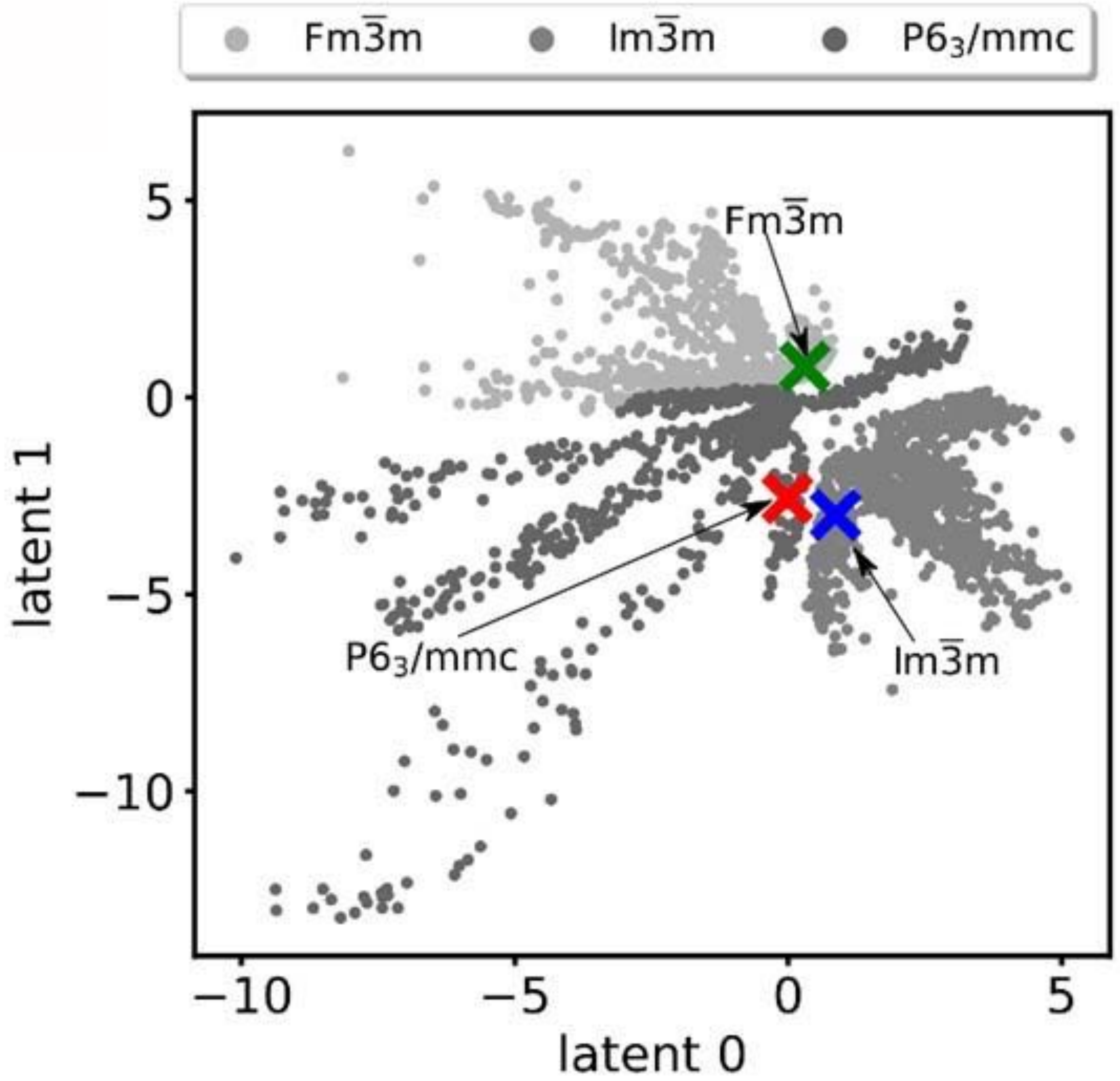




Maffettone, P.M. *et al.*, *Nat. Comp. Sci.*, **1**, 290-297 (2021)

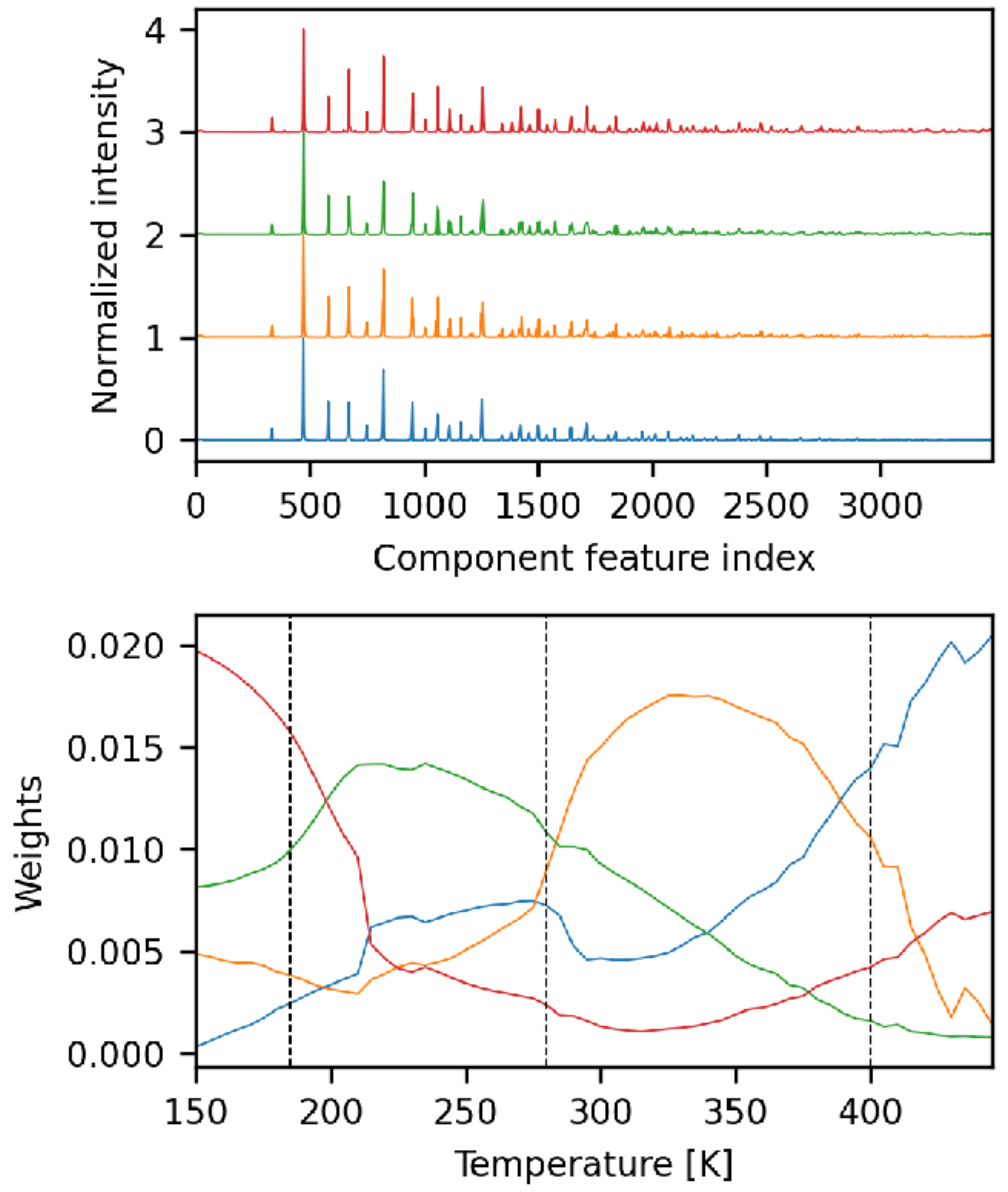
The latent space of variational auto encoders conditioned on the same synthetic dataset is a guide for novelty.





Banko, L. *et al.*, *npj. Comp. Matter.*, ***7***, 104 (2021)

Non-negative matrix factorization (NMF) for decomposing datasets without priors.



$\mathbf{X} \sim \mathbf{WH}$

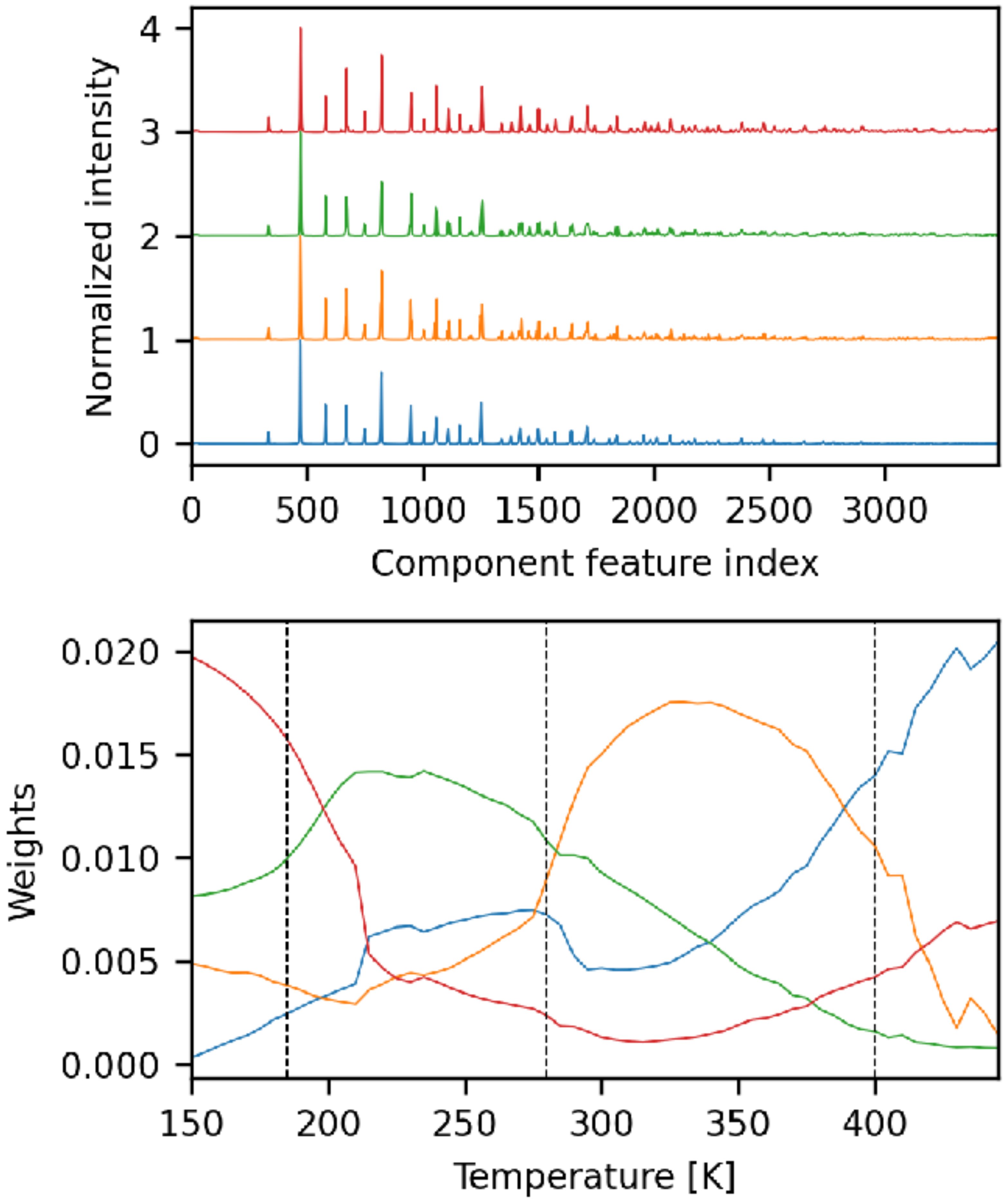
W (m patterns, k components)

H (k components, n features)

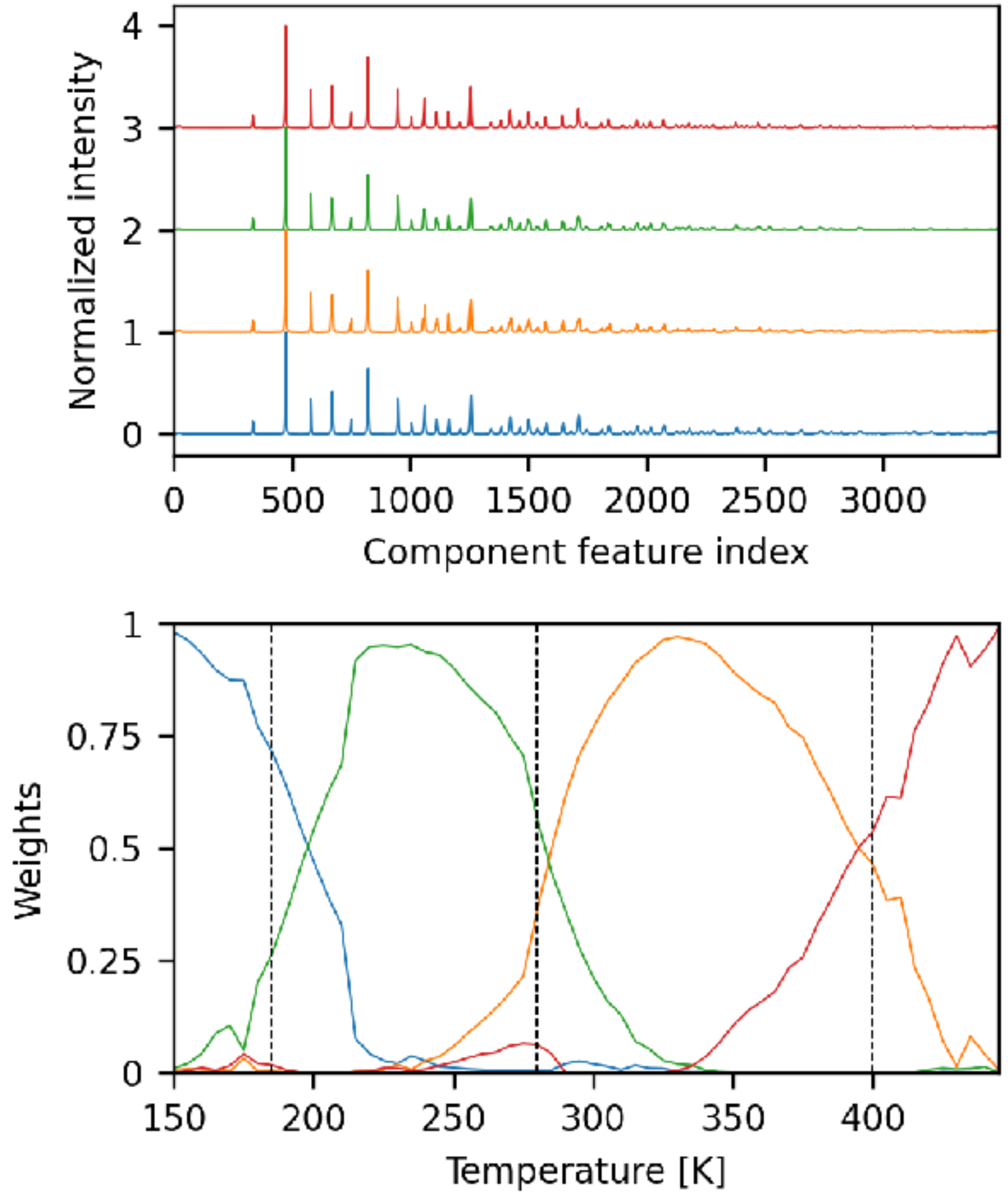
Appl. Phys. Rev. **Accepted** (arXiv:2104.00864)

Constrained NMF produces physically realistic components and weights.

Canonical



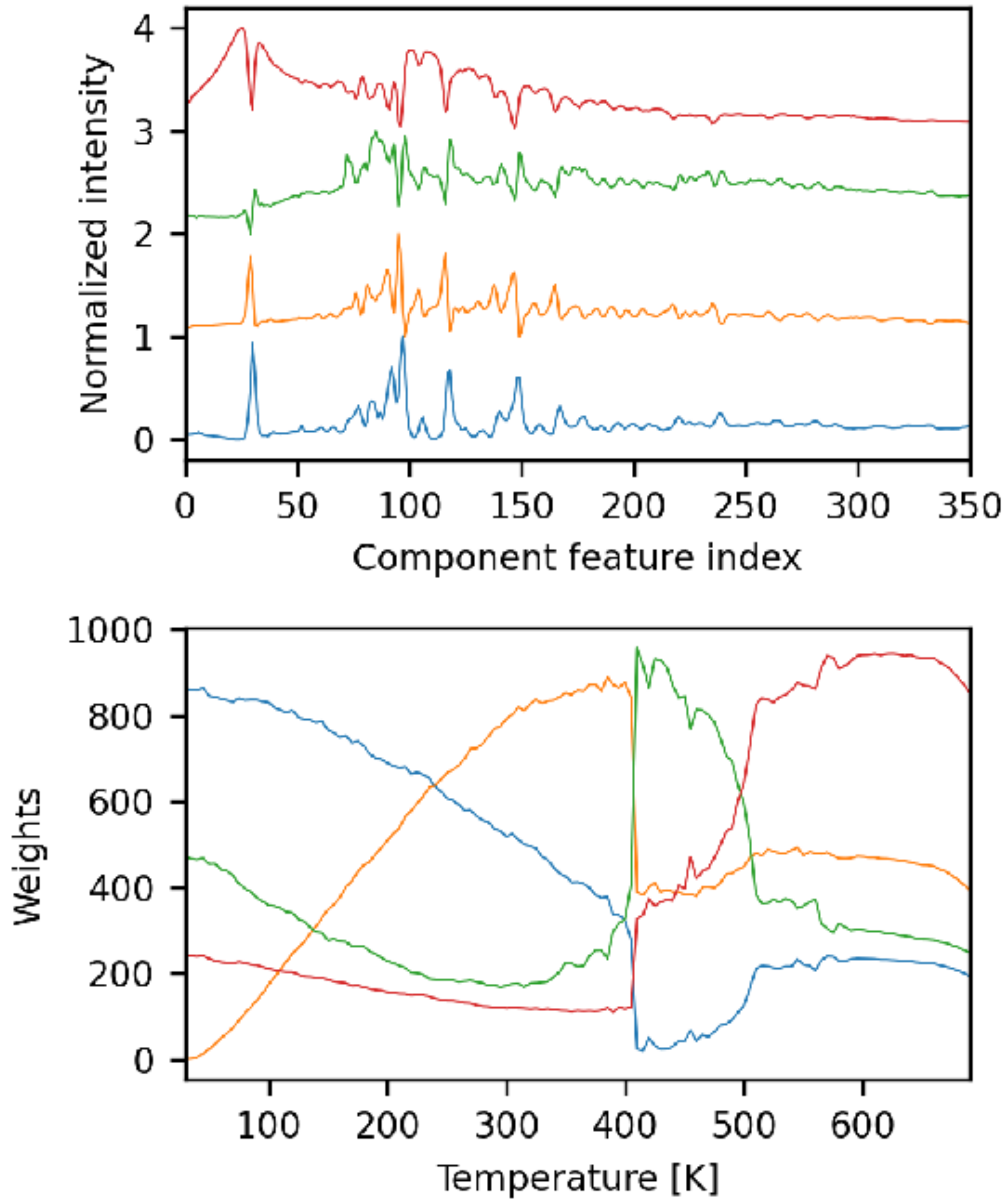
Constrained



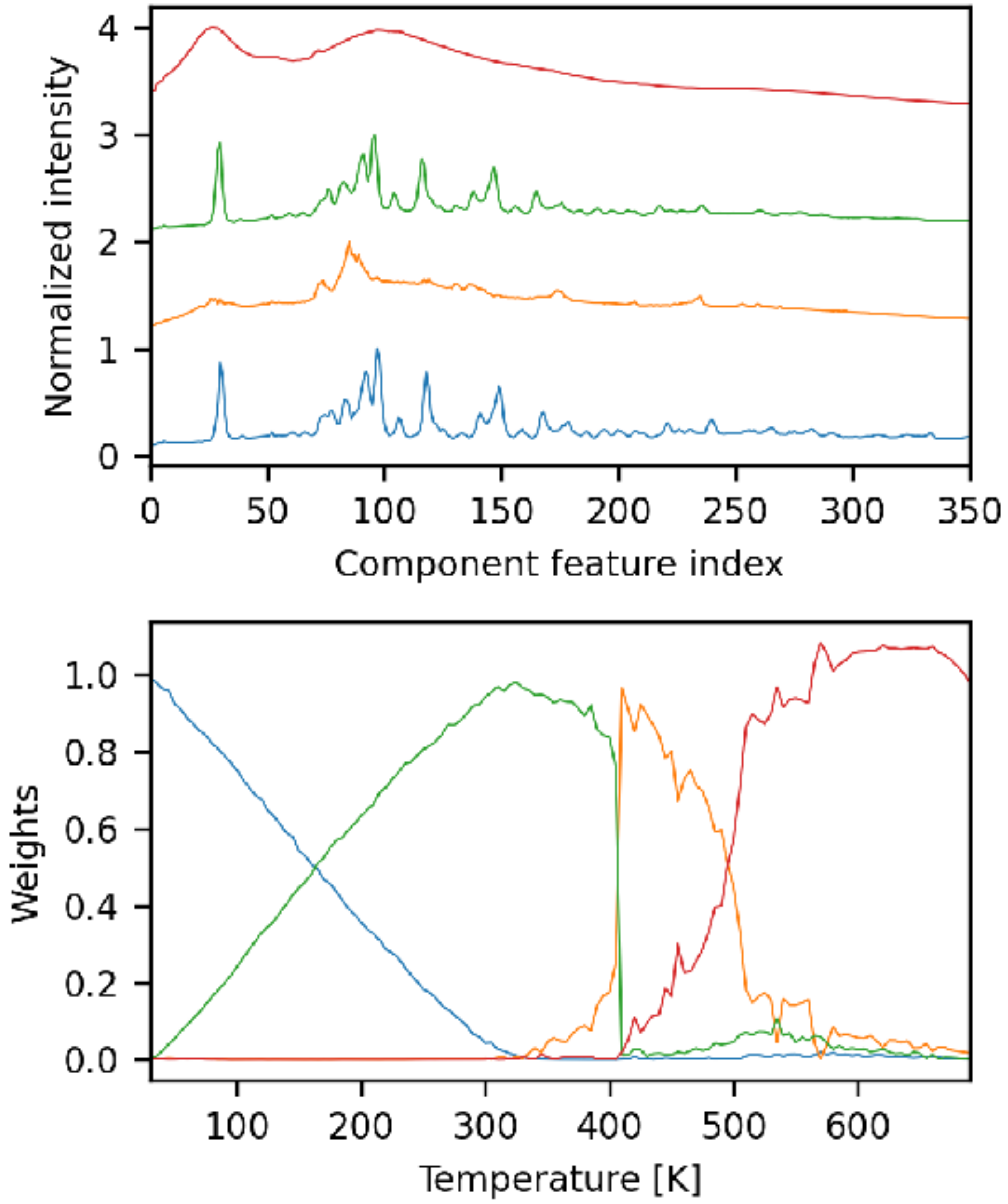
Appl. Phys. Rev. **Accepted** (arXiv:2104.00864)

Dynamically adjusted constraints leads to directly interpretable decompositions

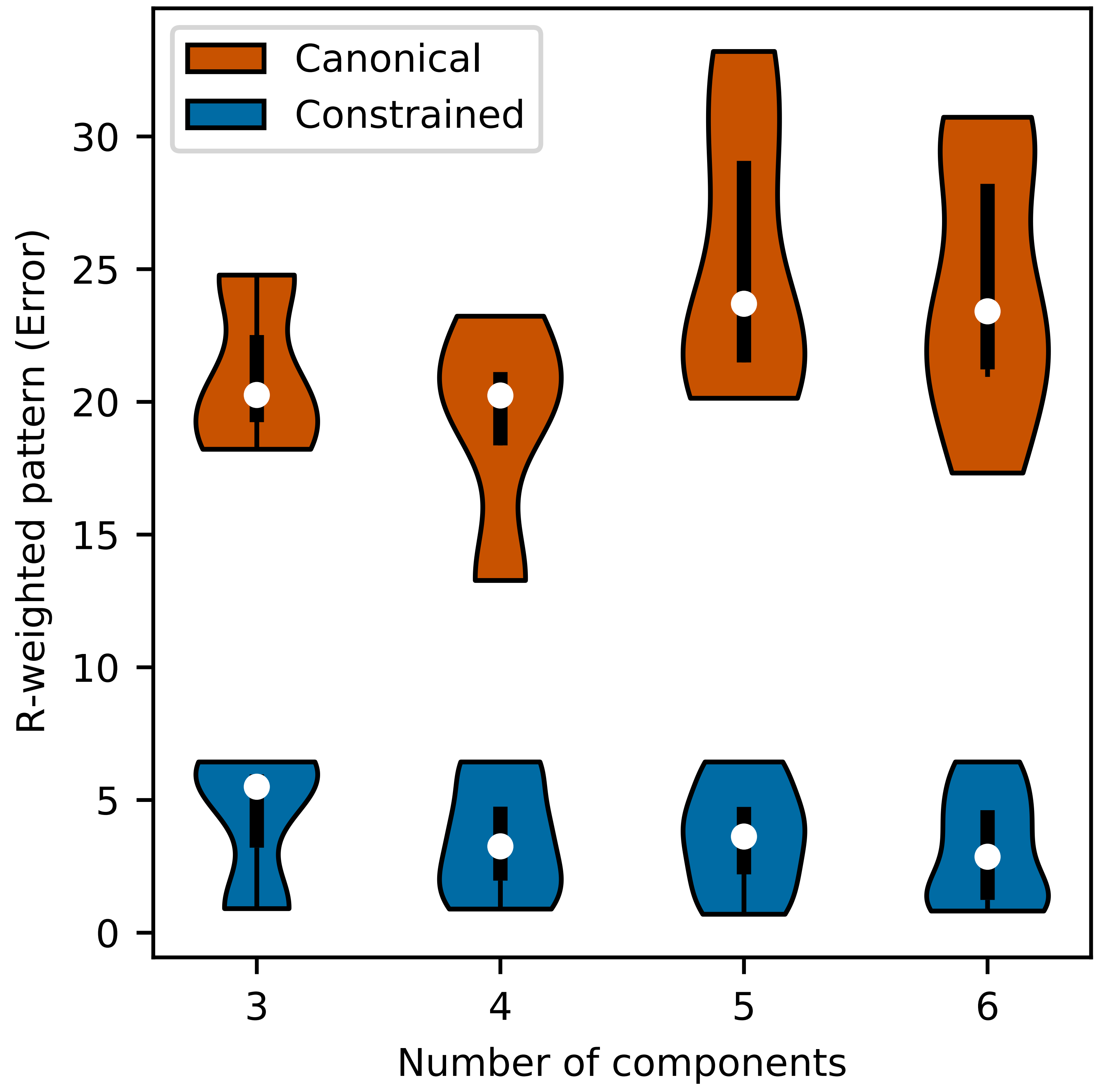
Canonical



Constrained



Refinement Results



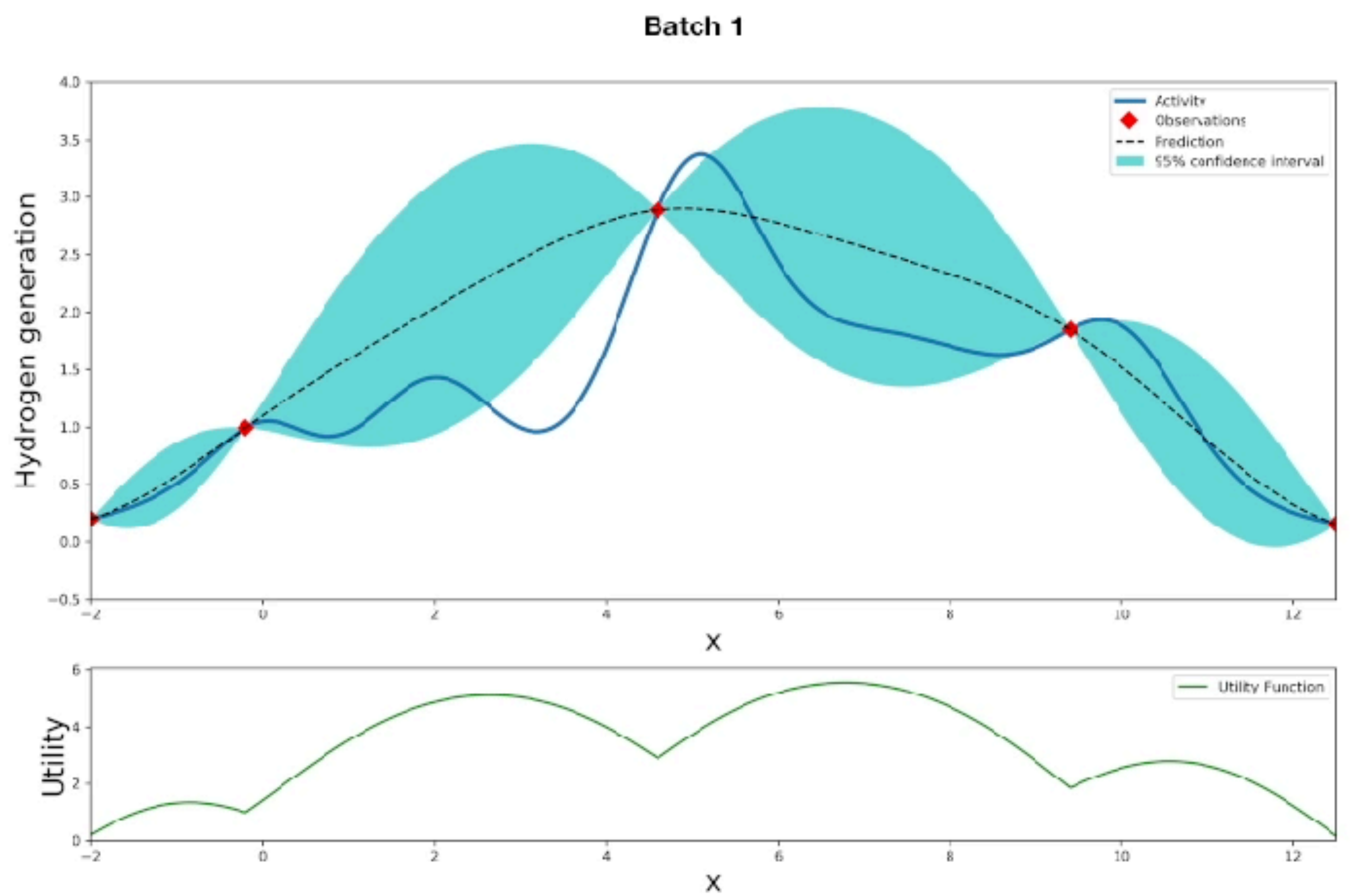
Appl. Phys. Rev. **Accepted** (arXiv:2104.00864)

Making decisions on what to measure next:

Active learning for exploring phase space

Reinforcement learning for operating under resource constraints

Bayesian optimization to guide experiments.



1. Prescribe a prior belief (Gaussian).
2. Calculate the posterior probability.
3. Use an acquisition function based on the posterior.
4. Sample the acquisition function according to the batch size and greed.

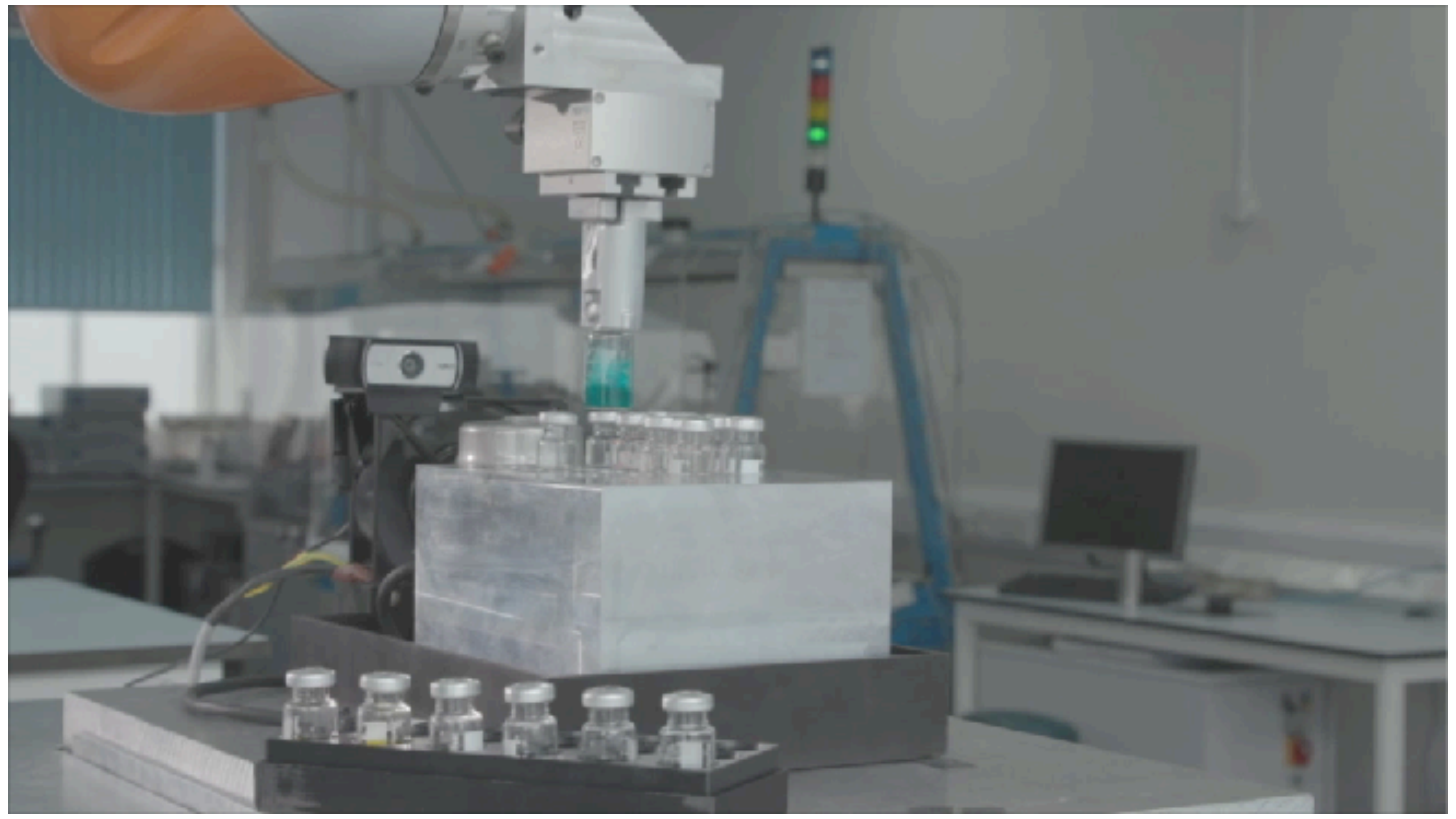
Nature **583**, 237-241 (2020)

Autonomous discovery

Solid dispensing

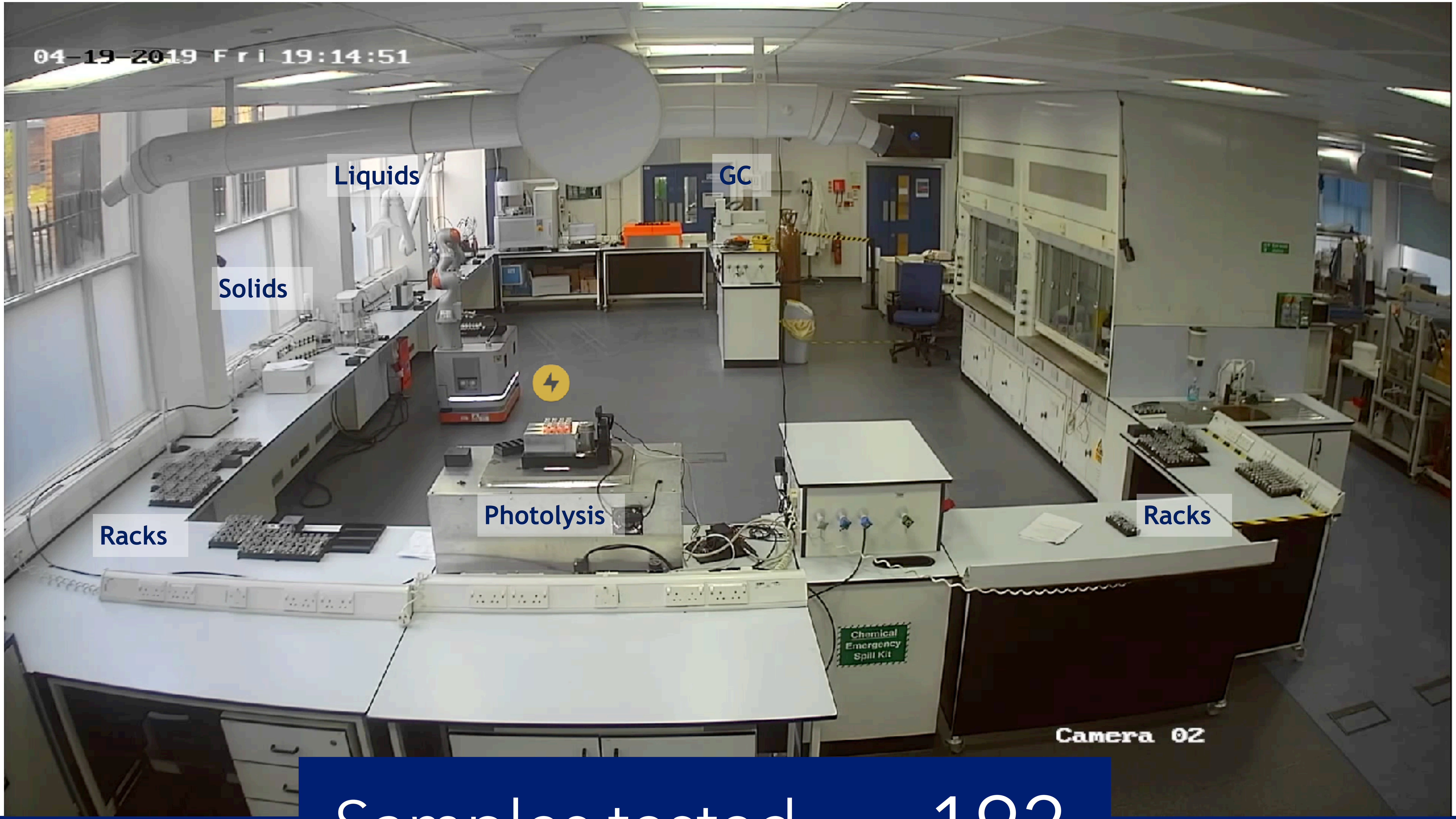
Liquid dispensing
Inertization

Photolysis



Measurement

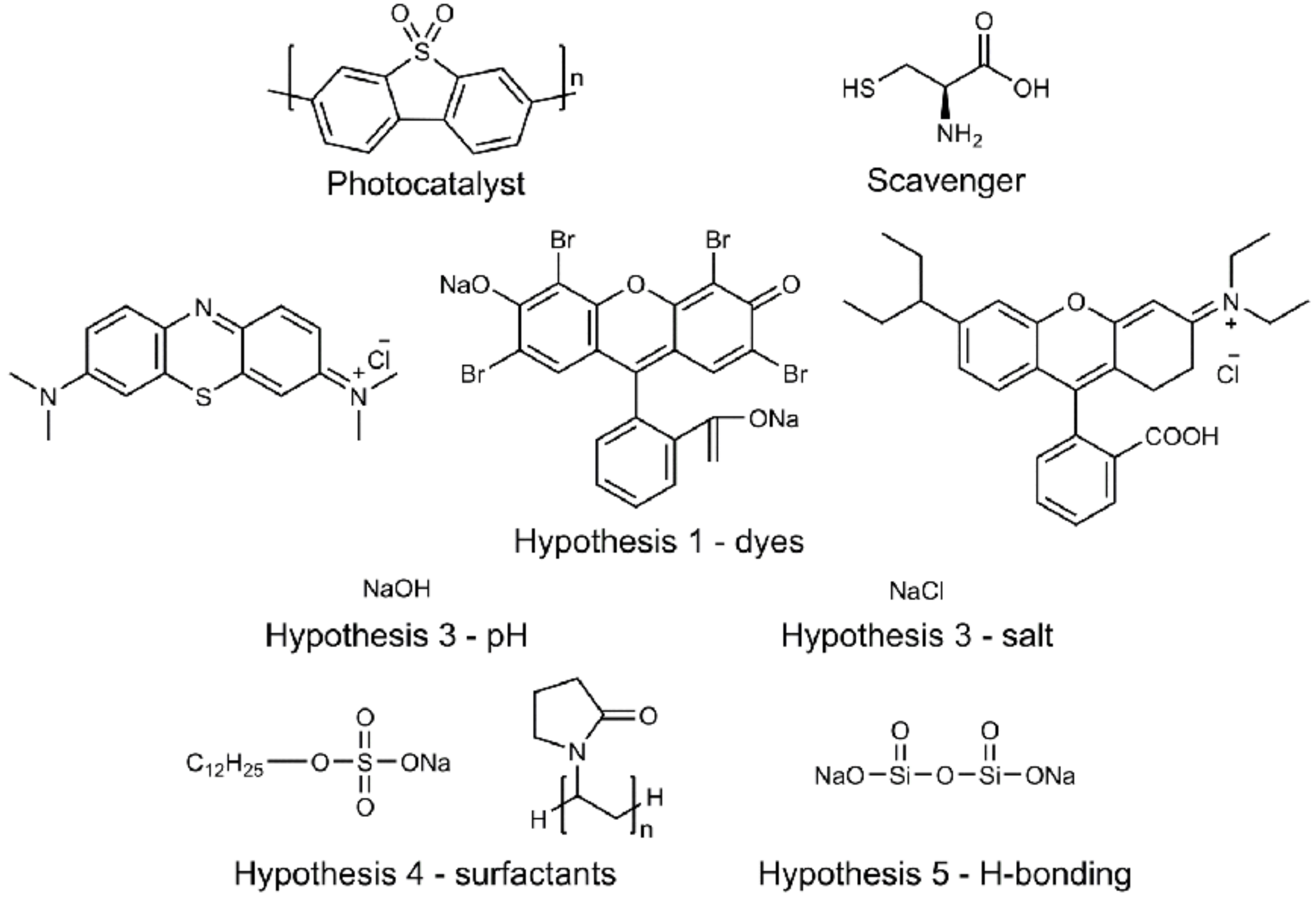
48 hours of research in 60 seconds

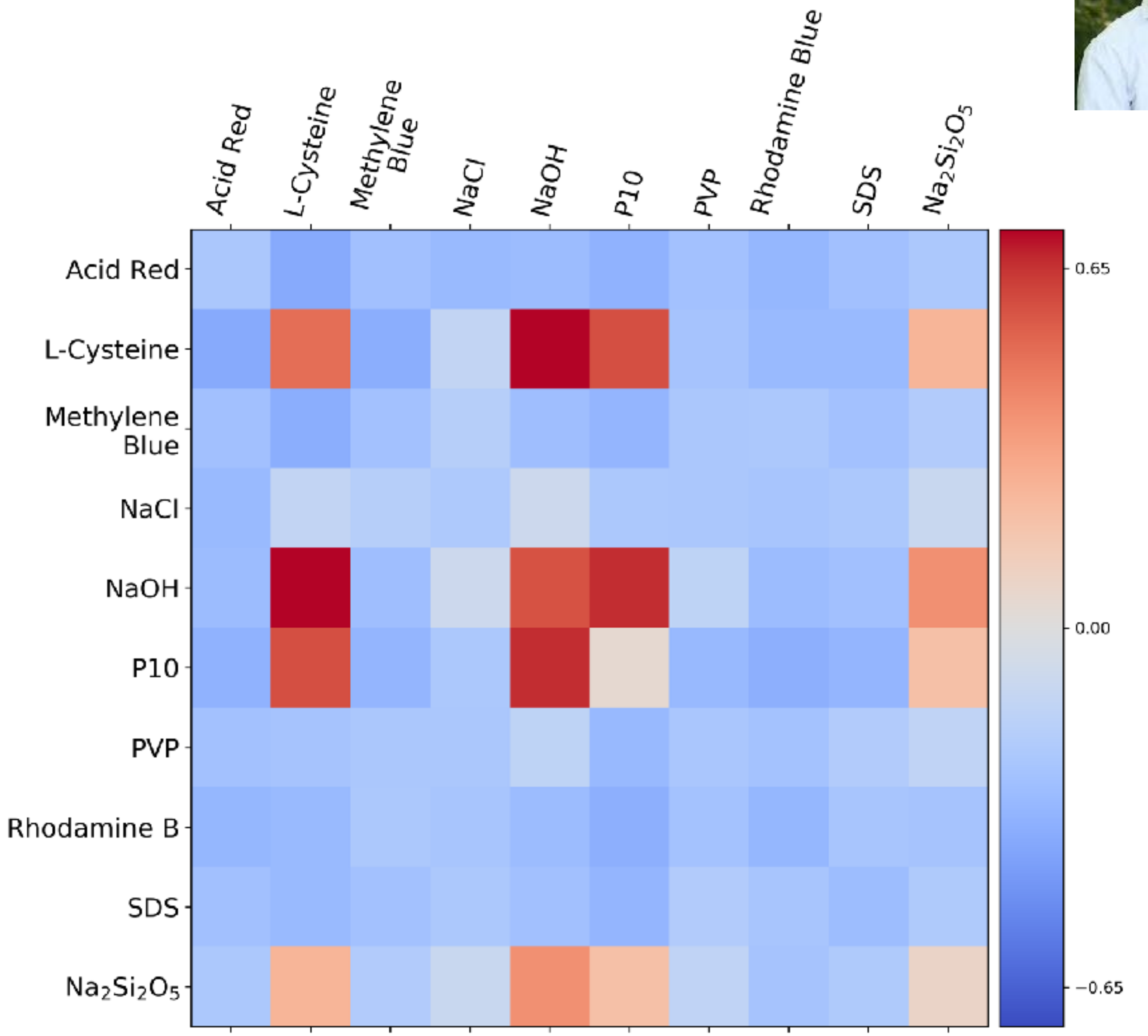


Samples tested = 192

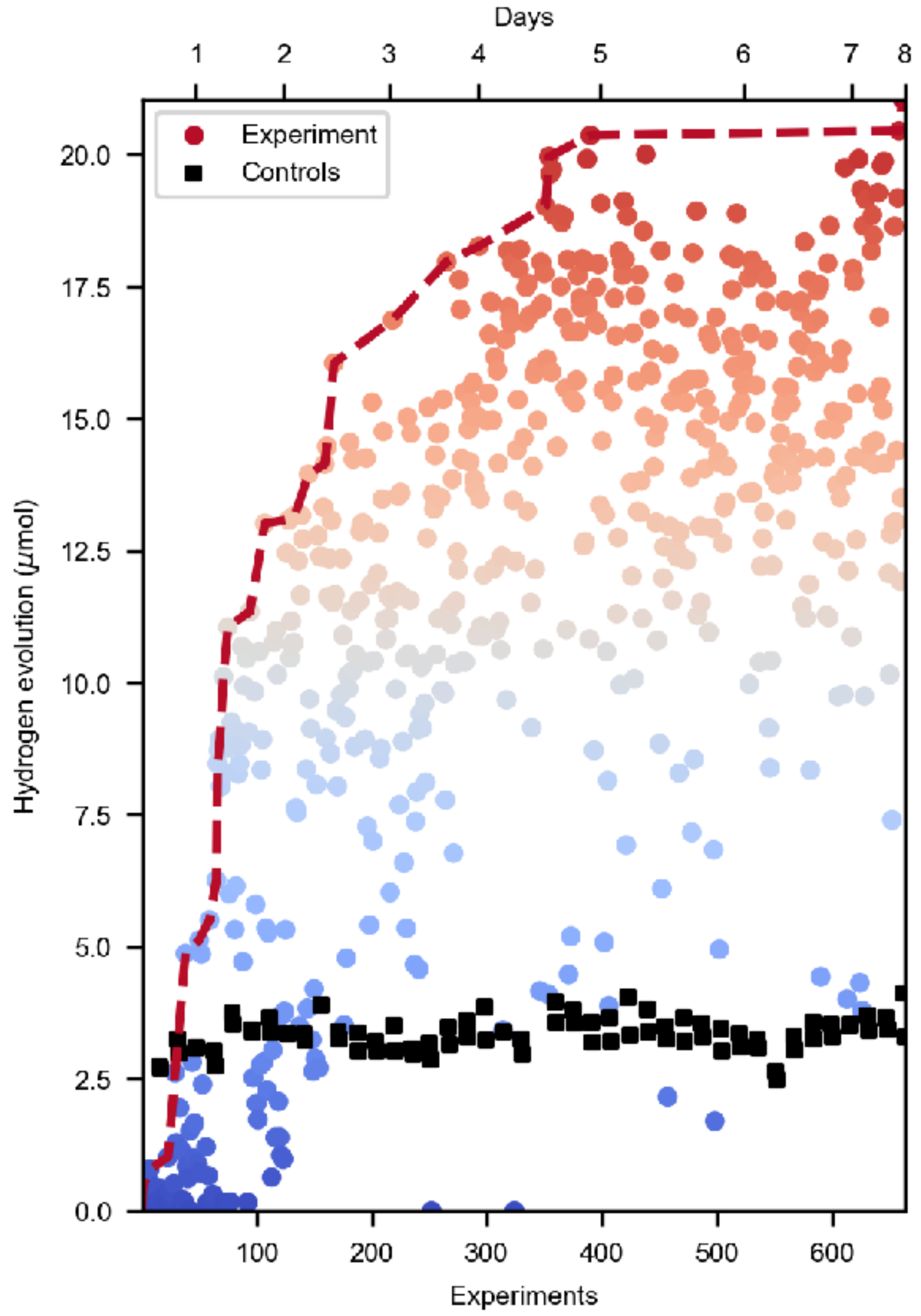
Nature **583**, 237-241 (2020).

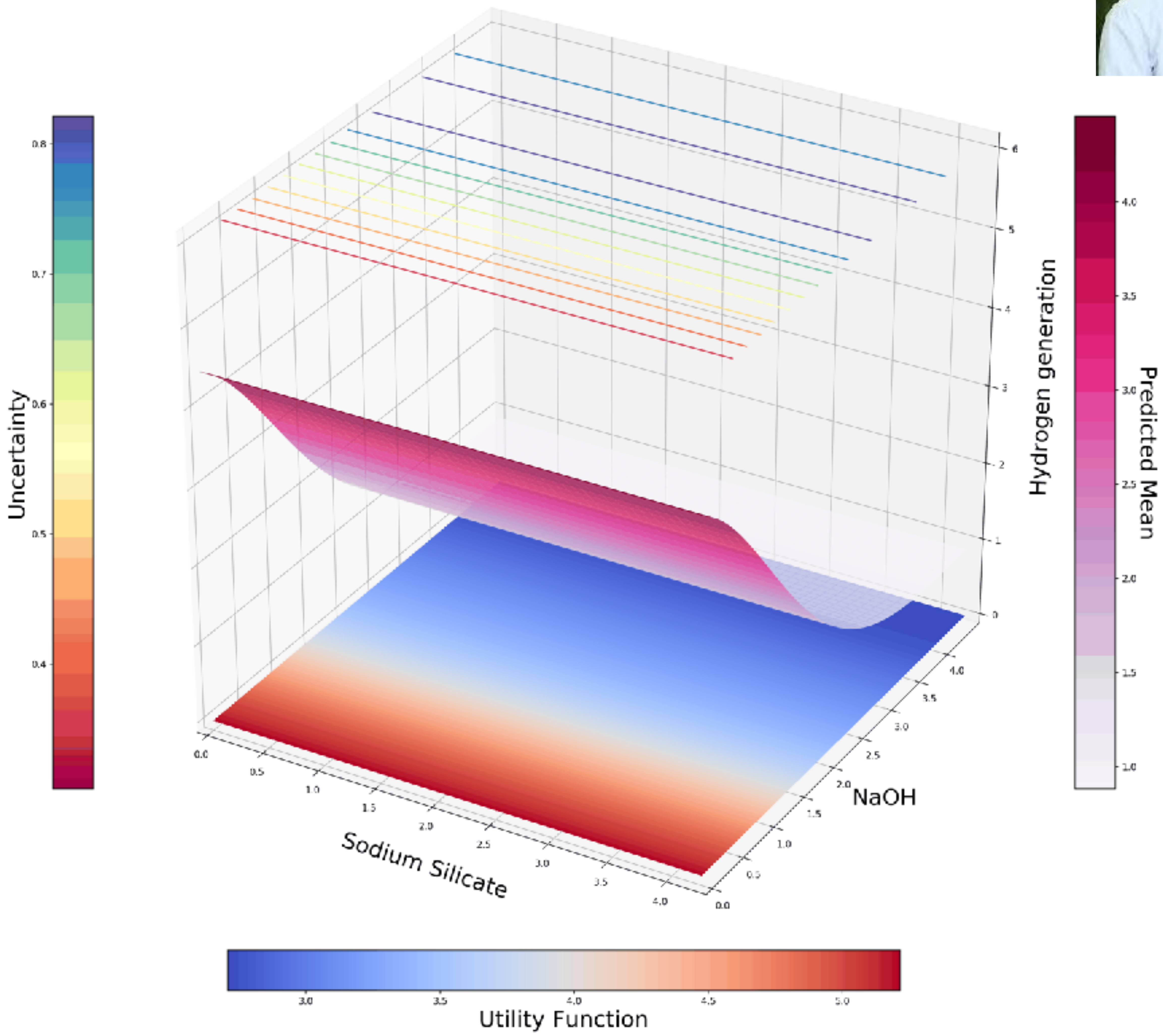
Human defined experiments ran by robot researchers



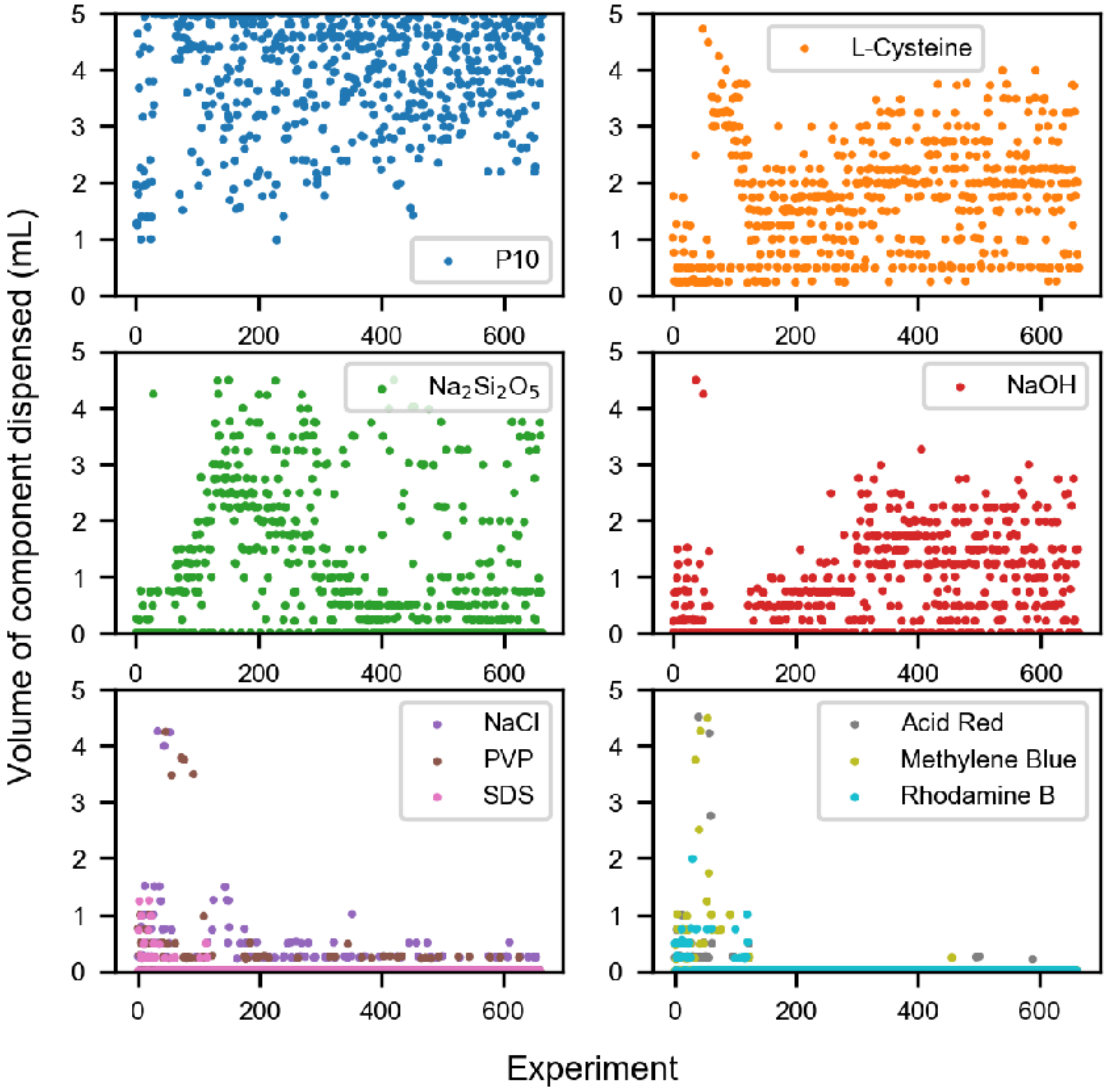


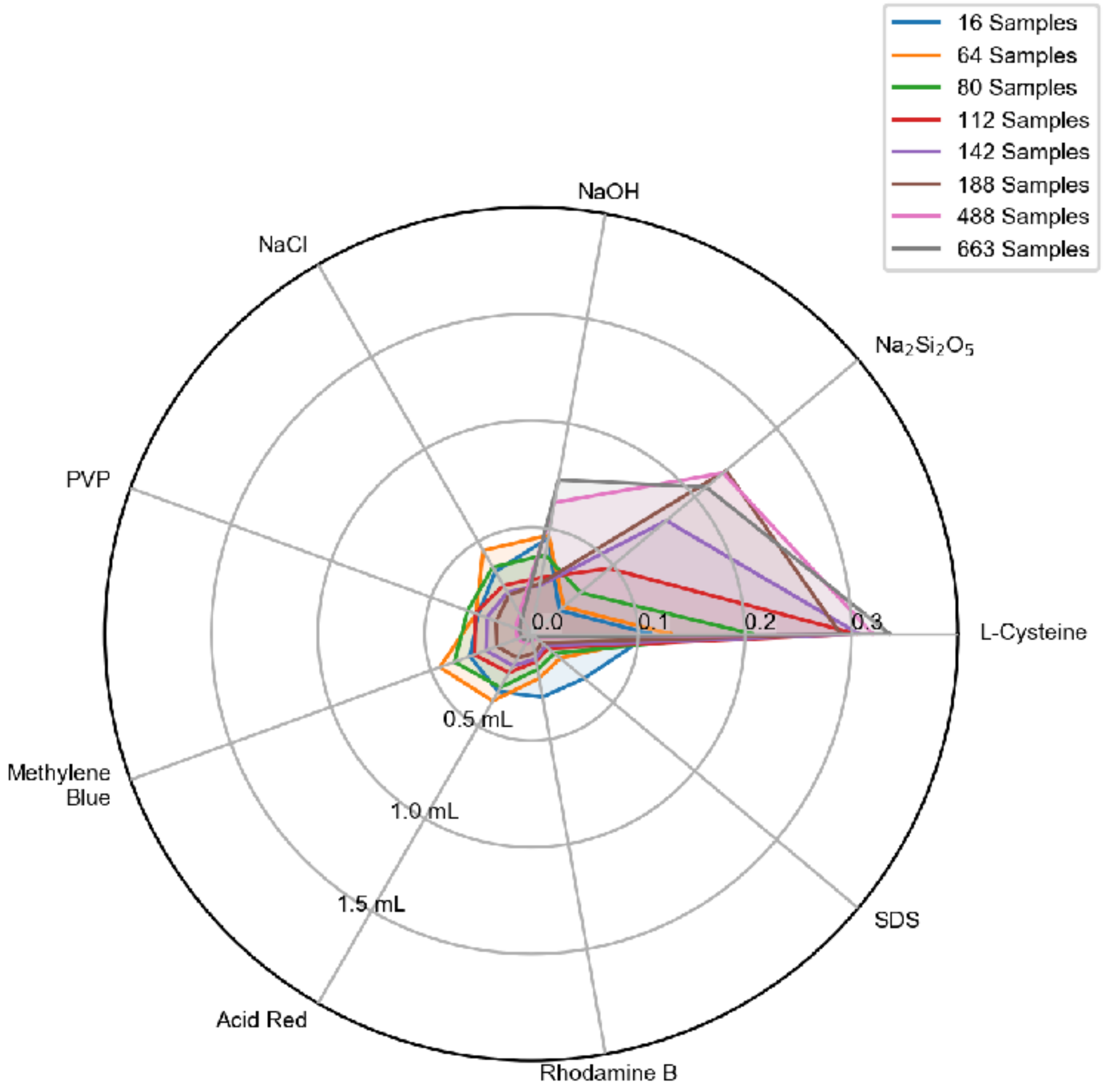
Models develop over time and balance exploration and exploitation





Important components are automatically selected





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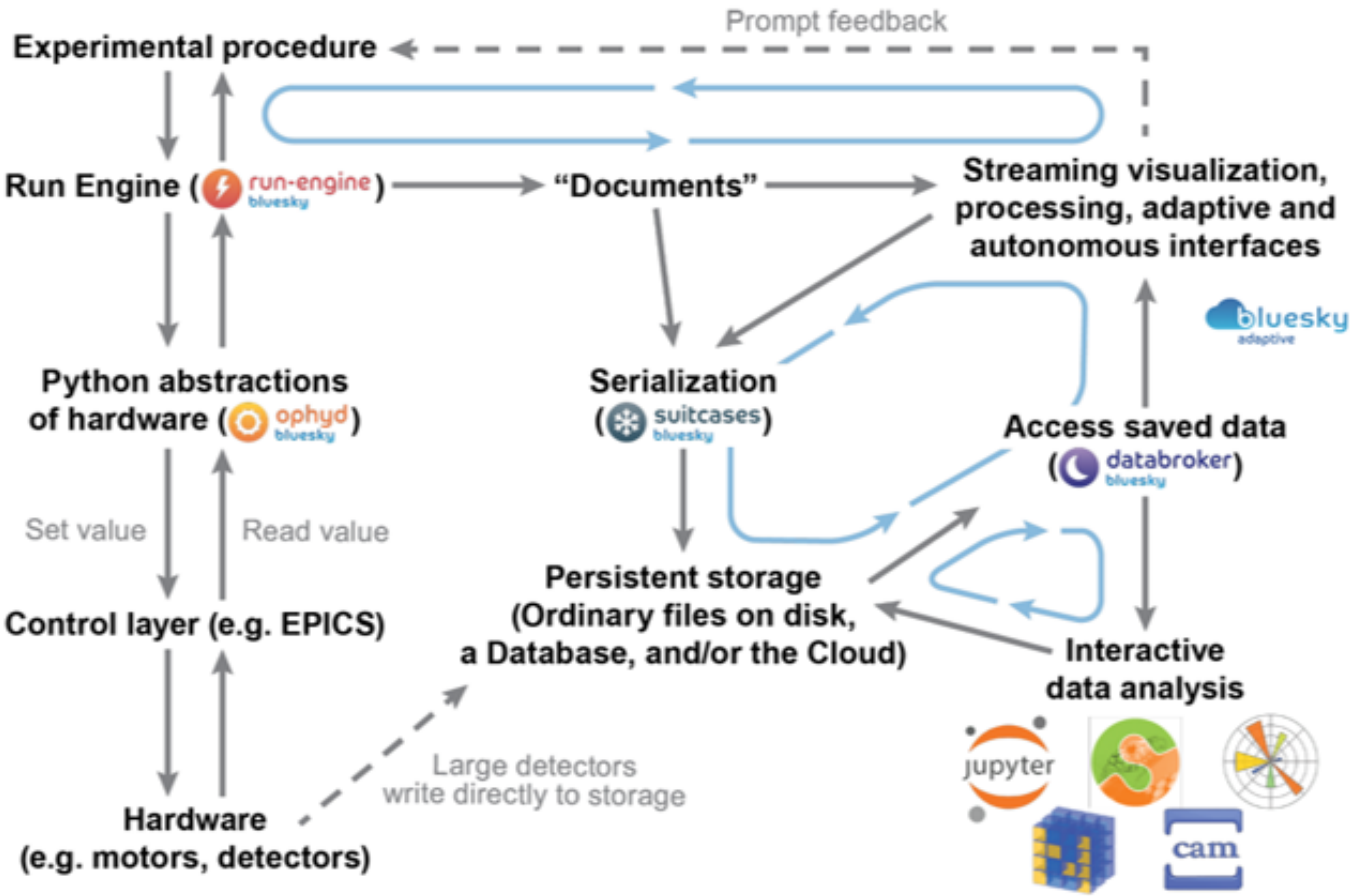
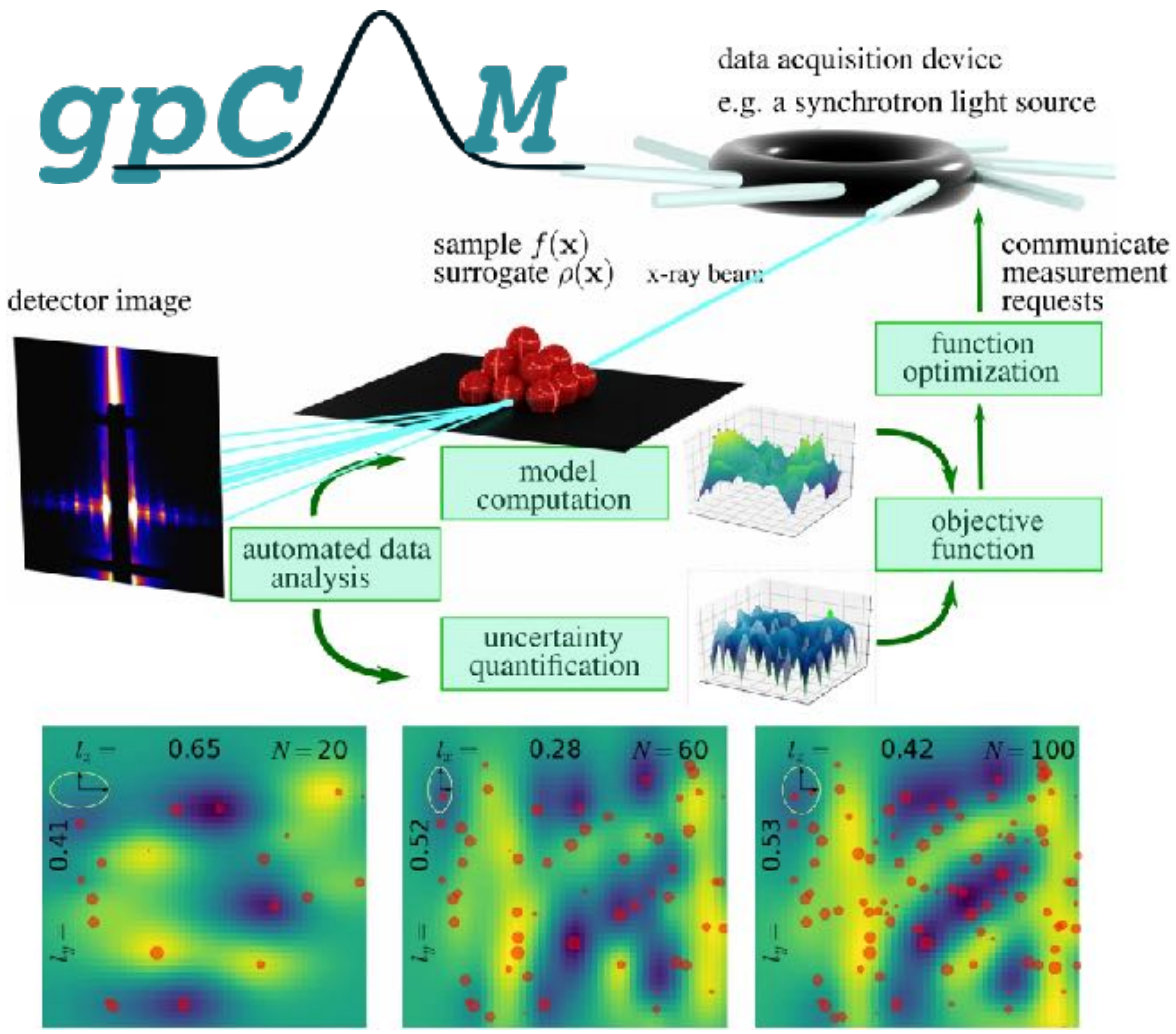
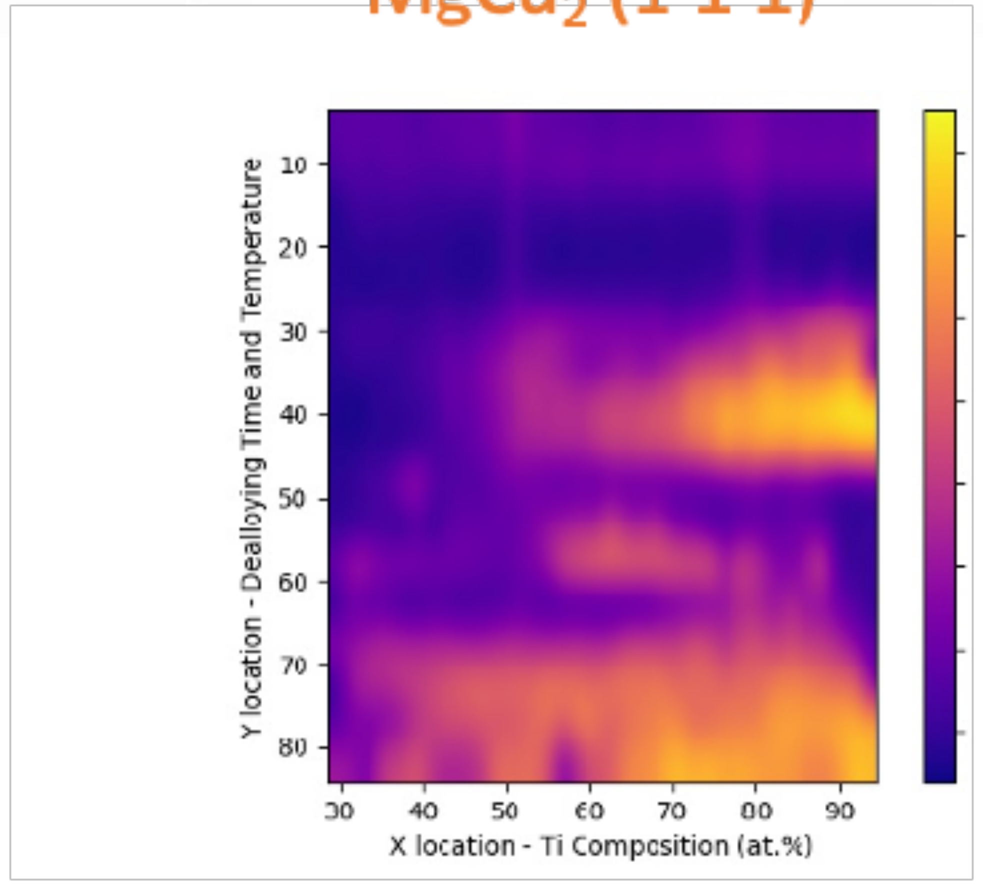
Bayesian optimization for autonomous characterization is enabled by bluesky-adaptive.



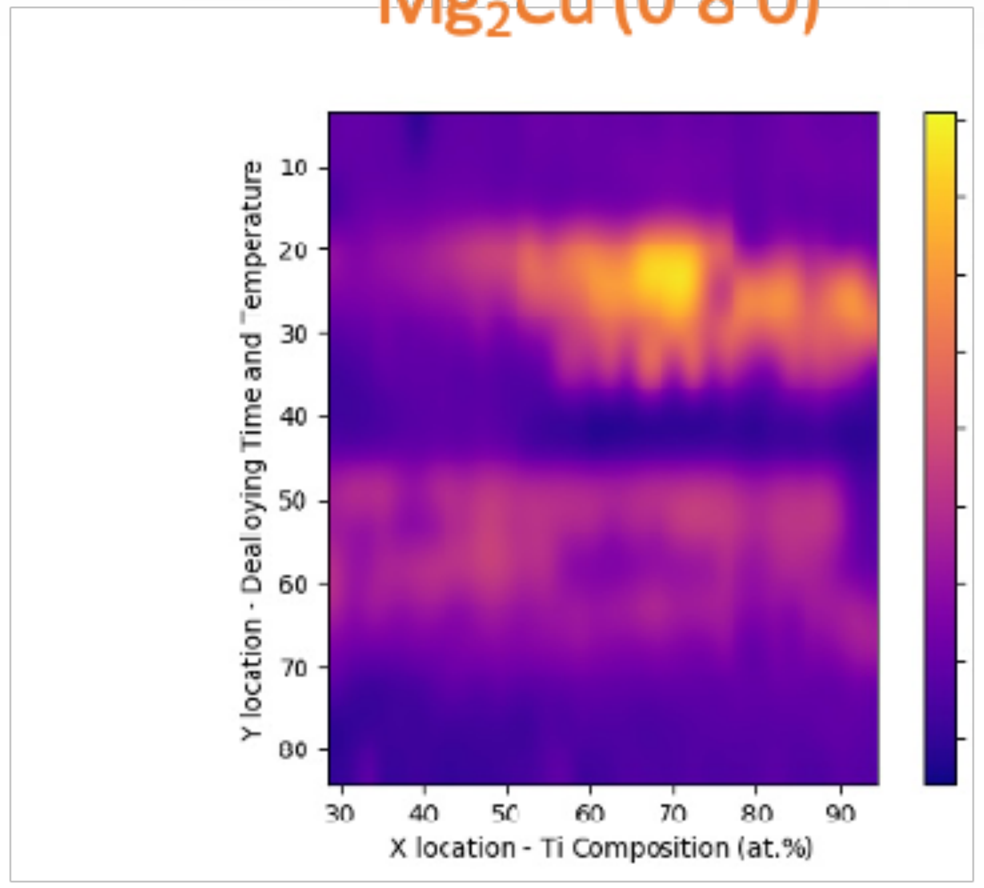


Probabilistic predictions from supervised models can also guide effective experimentation.

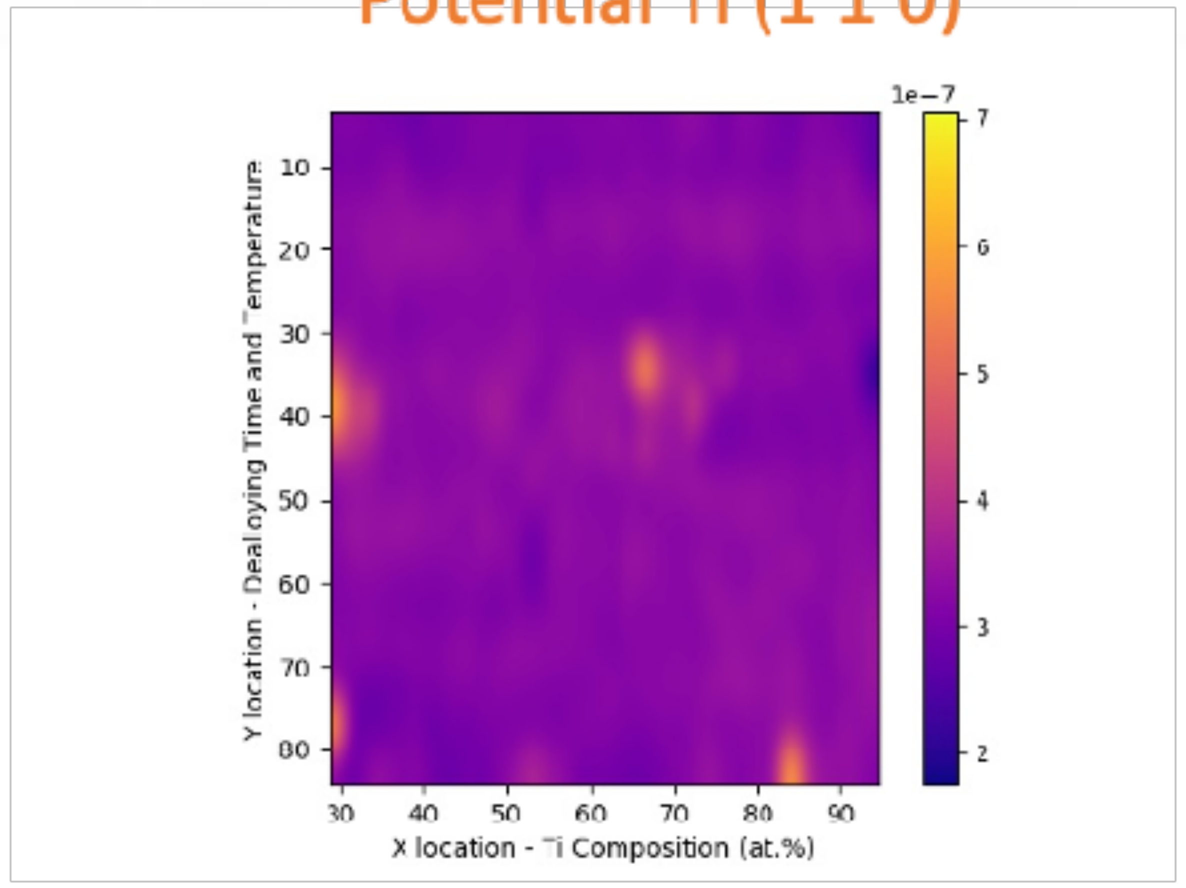
$MgCu_2$ (1 1 1)

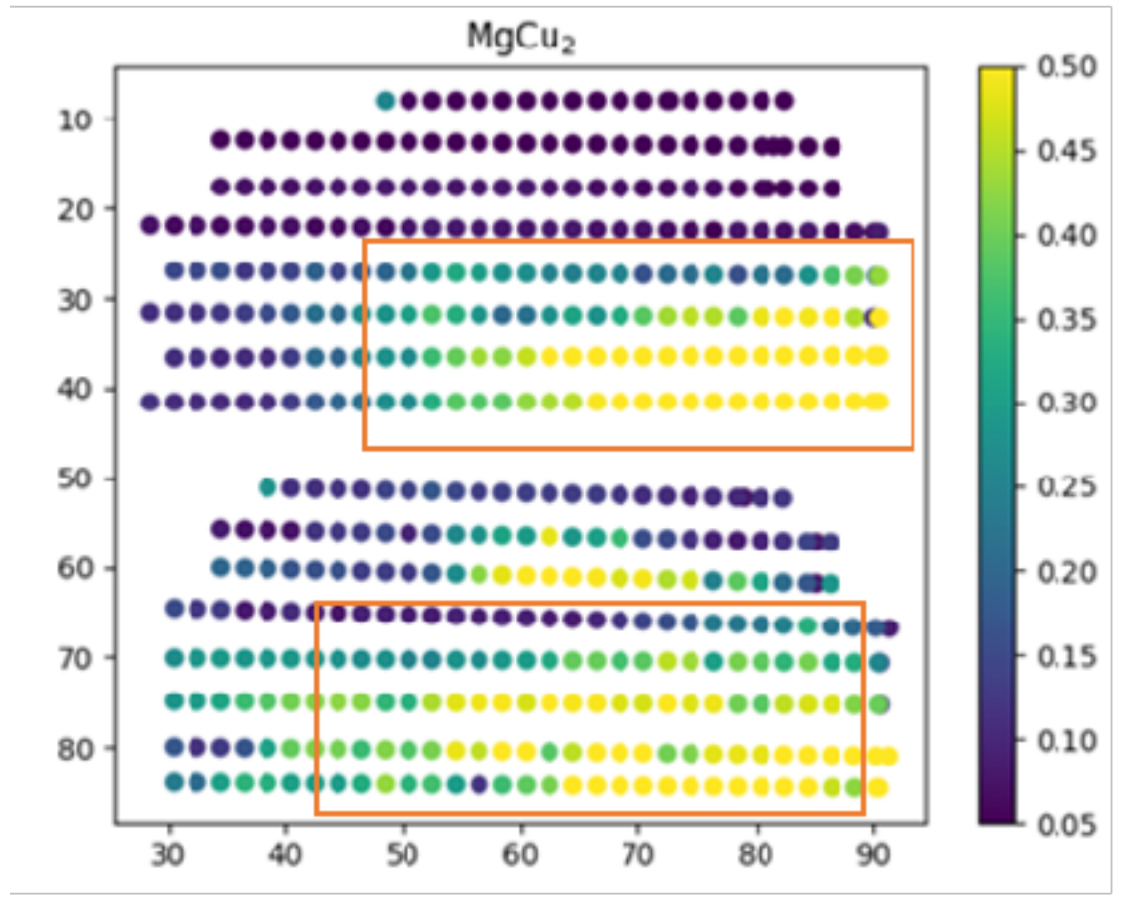


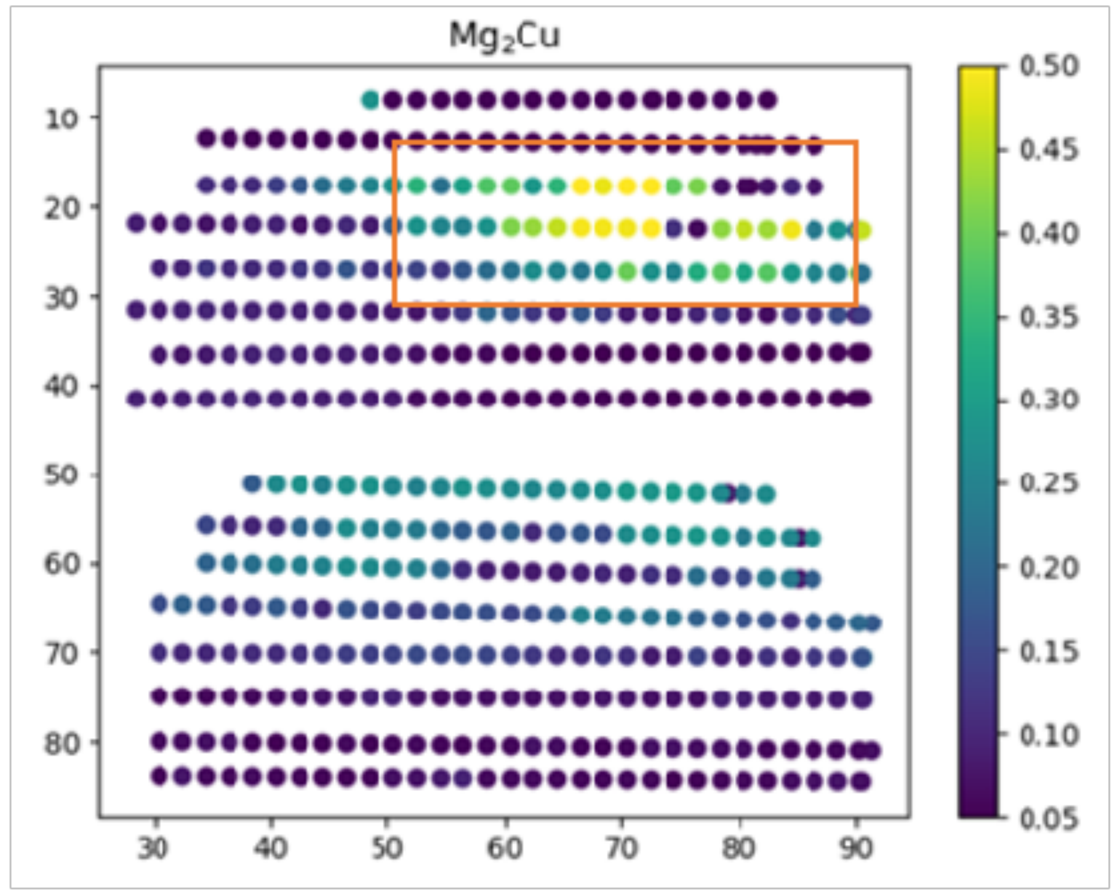
Mg_2Cu (0 8 0)

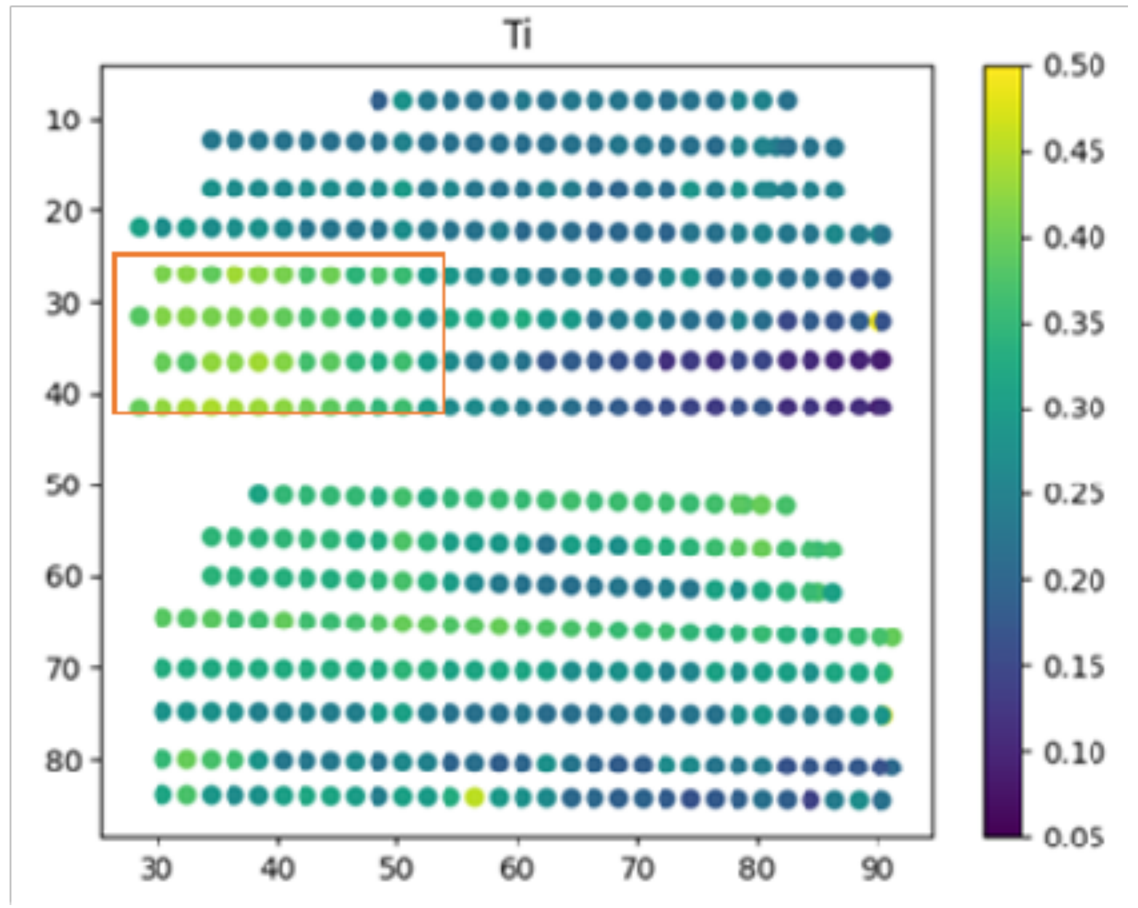


Potential Ti (1 1 0)









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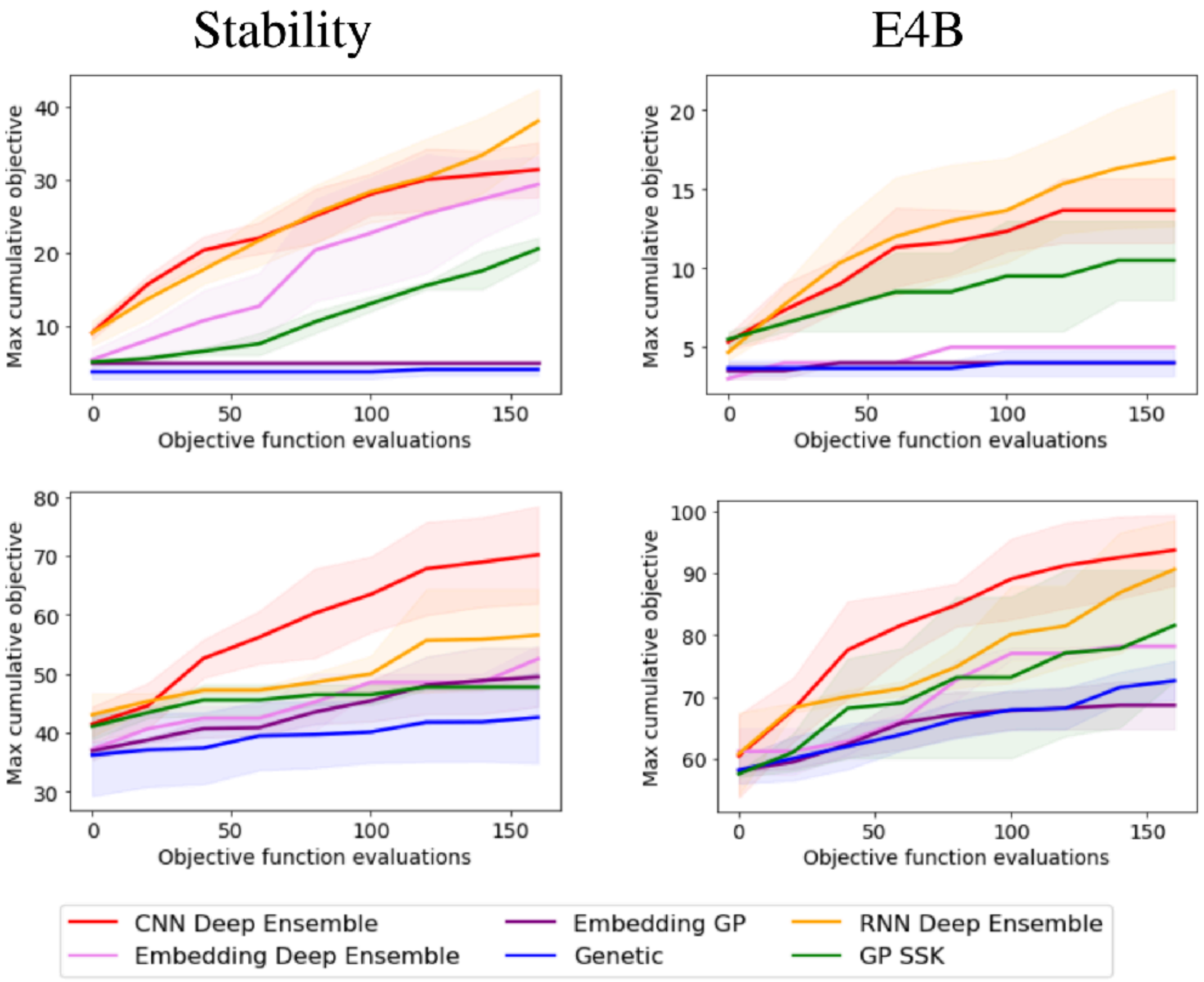
Stony Brook University

Under Review

National Synchrotron Light Source II

String based optimization tasks can be accomplished using a suite of network architectures.

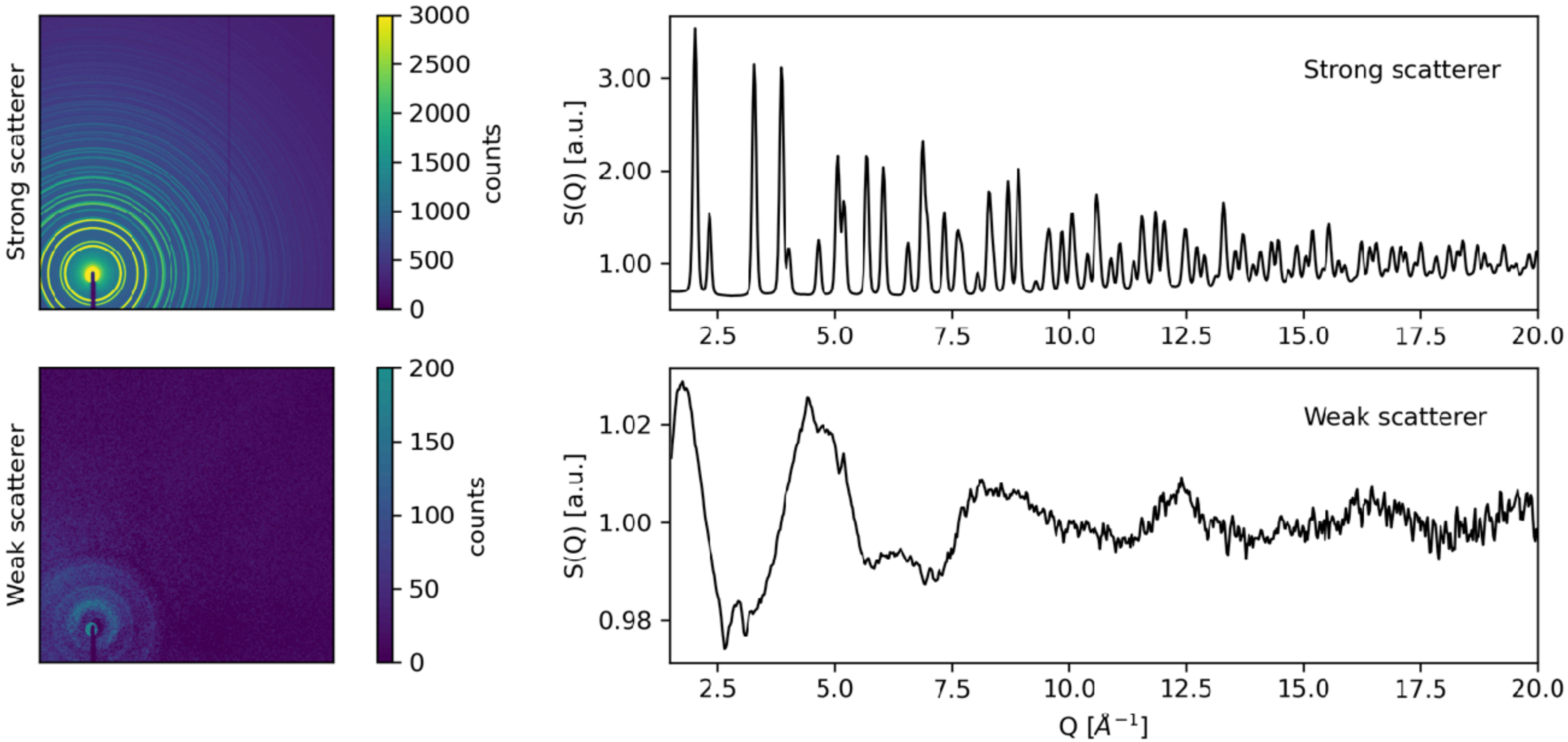


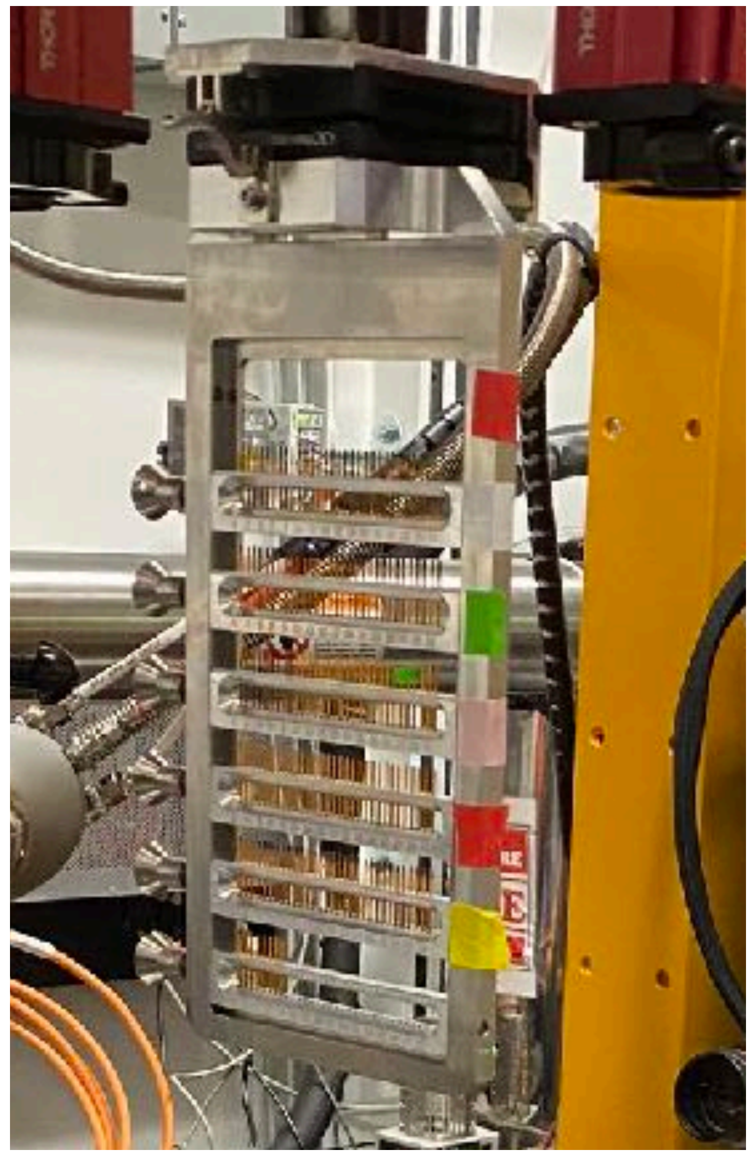
Gruver, N. *et al., ICML 2020*

Reinforcement learning:

For when model training is more costly than an experimental step.

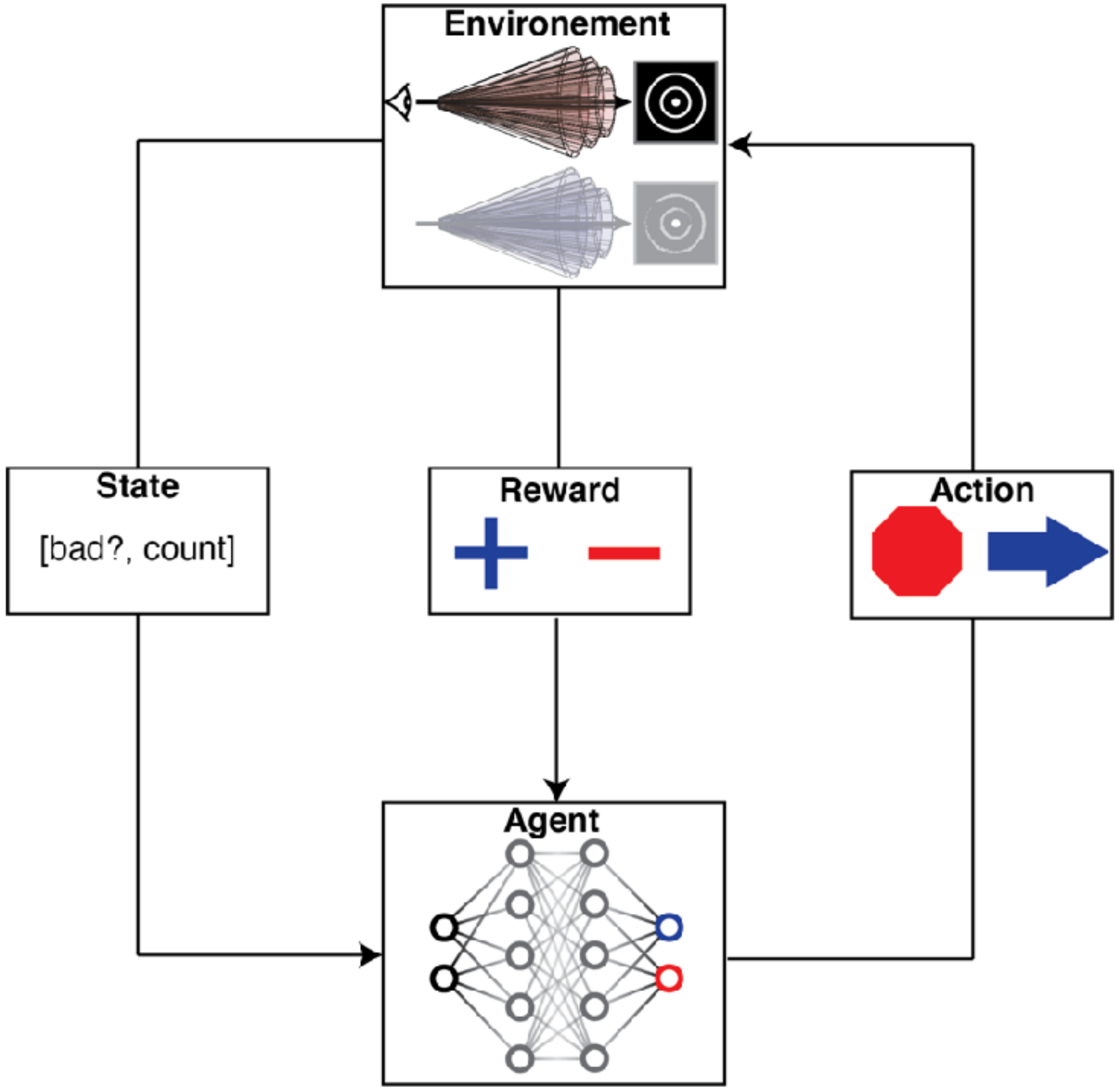
With hundreds of samples to run remotely, how do we best utilize our resources?

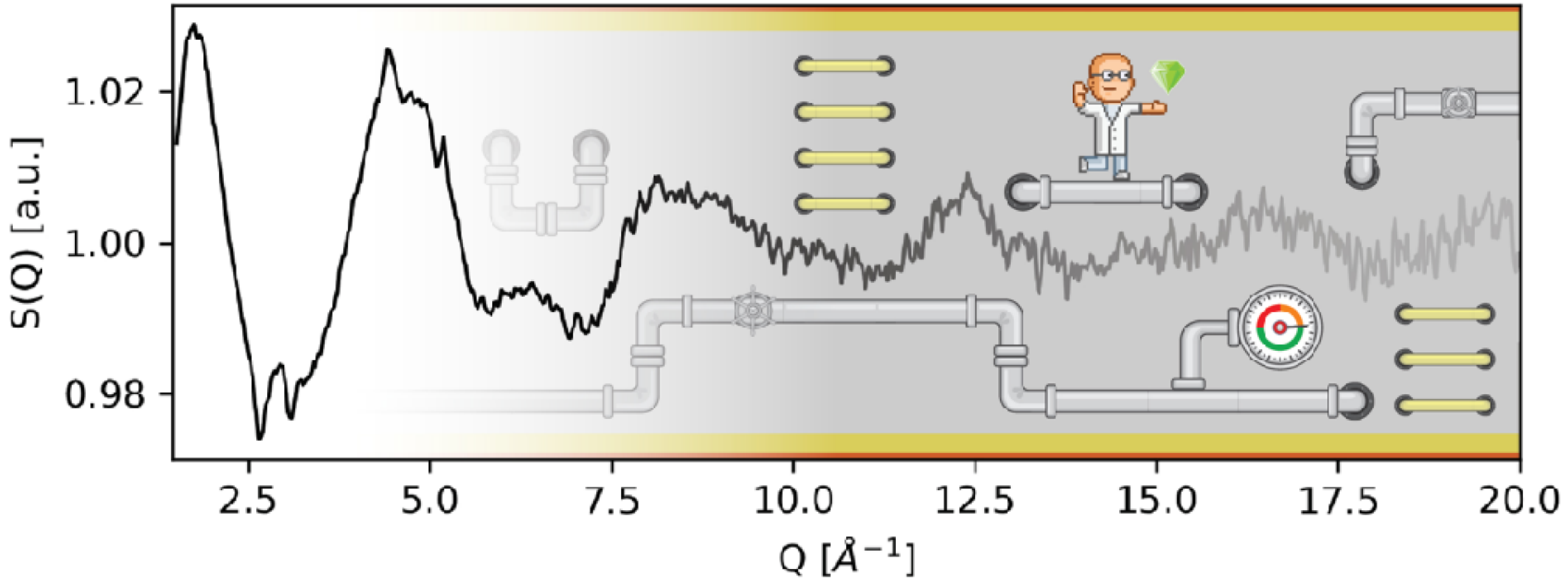




Mach. Learn.: Sci. Technol. **2**, 025025 (2021)

Reinforcement learning develops policies for optimal measurement strategies.





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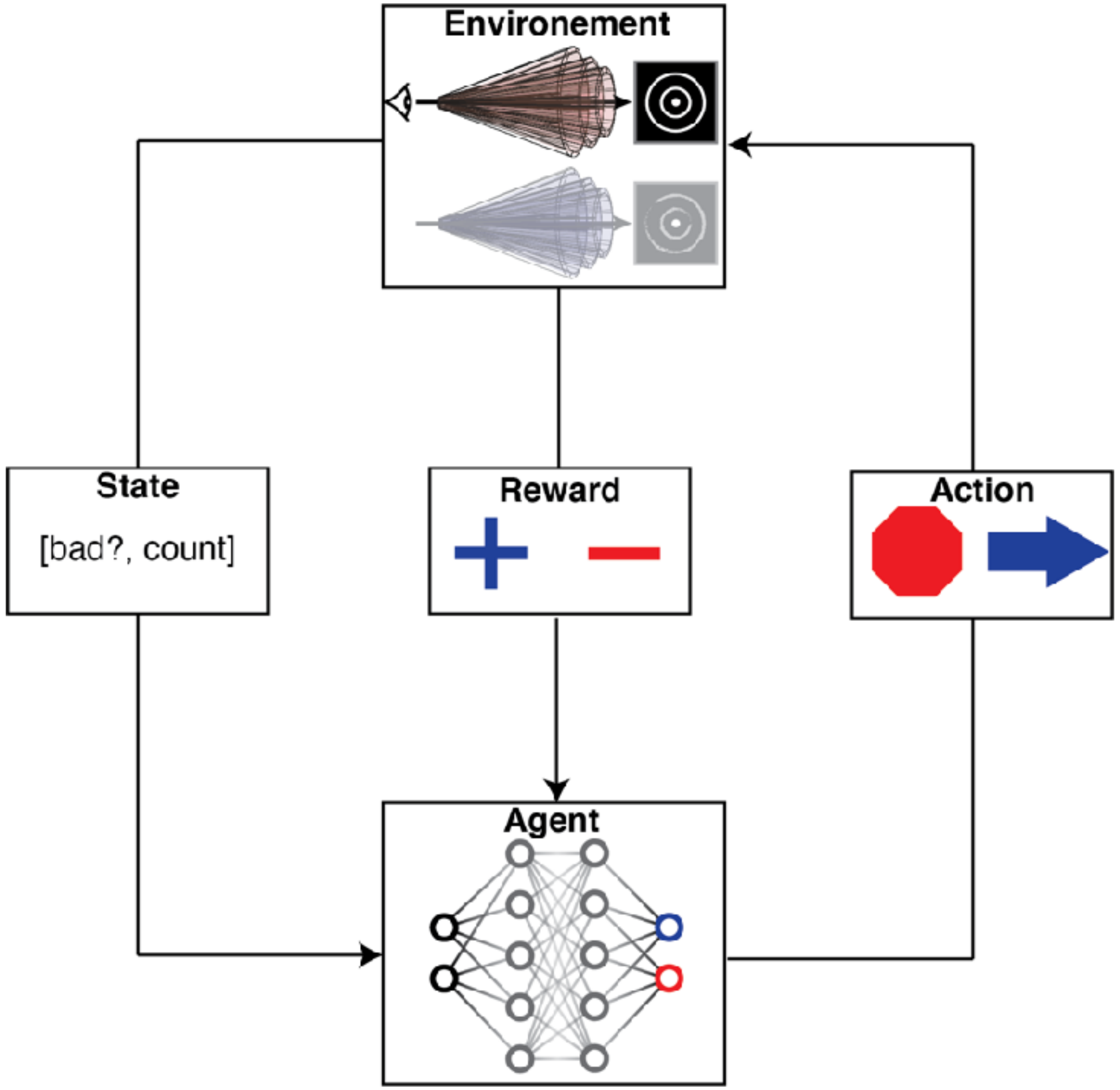
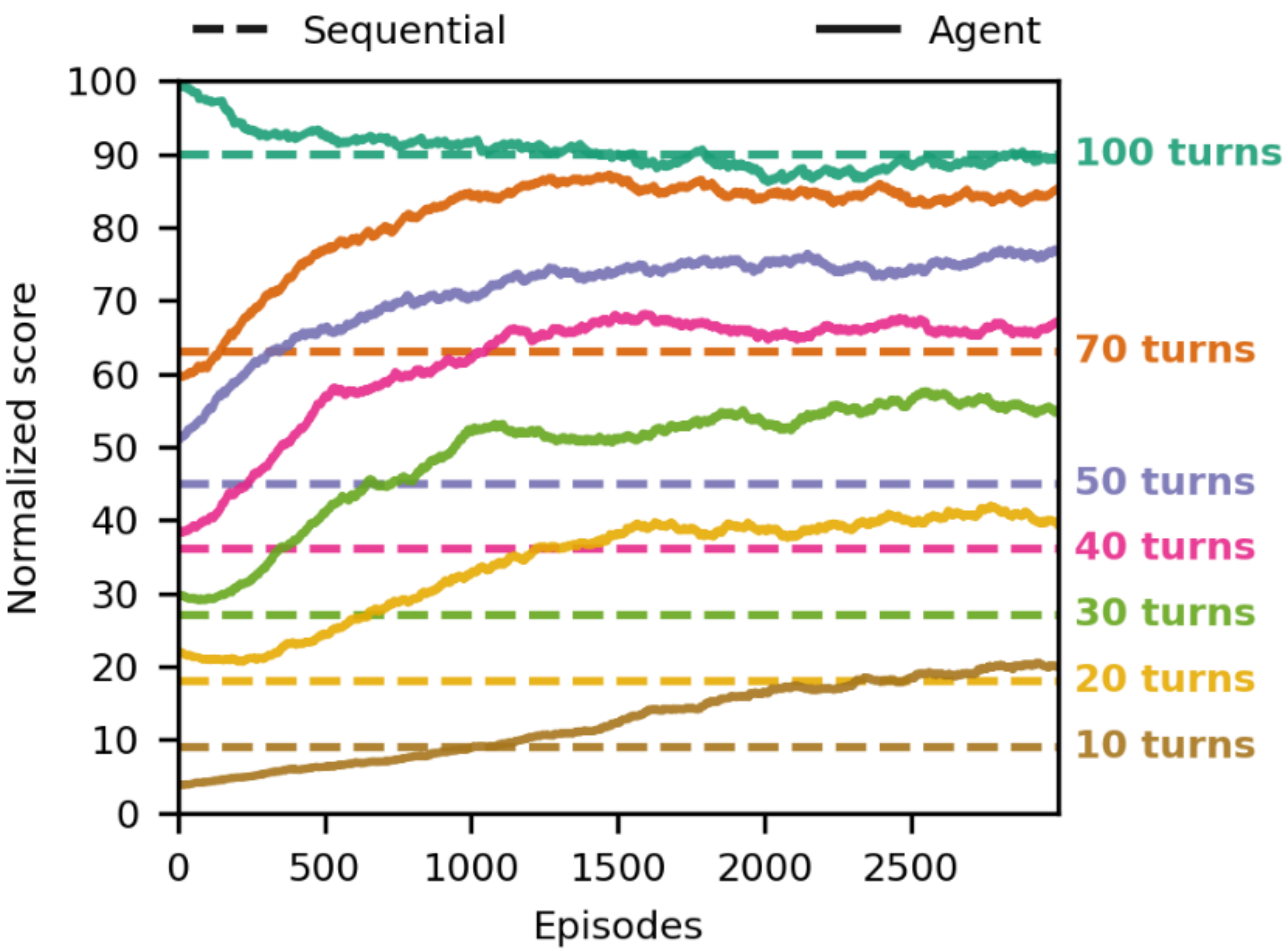
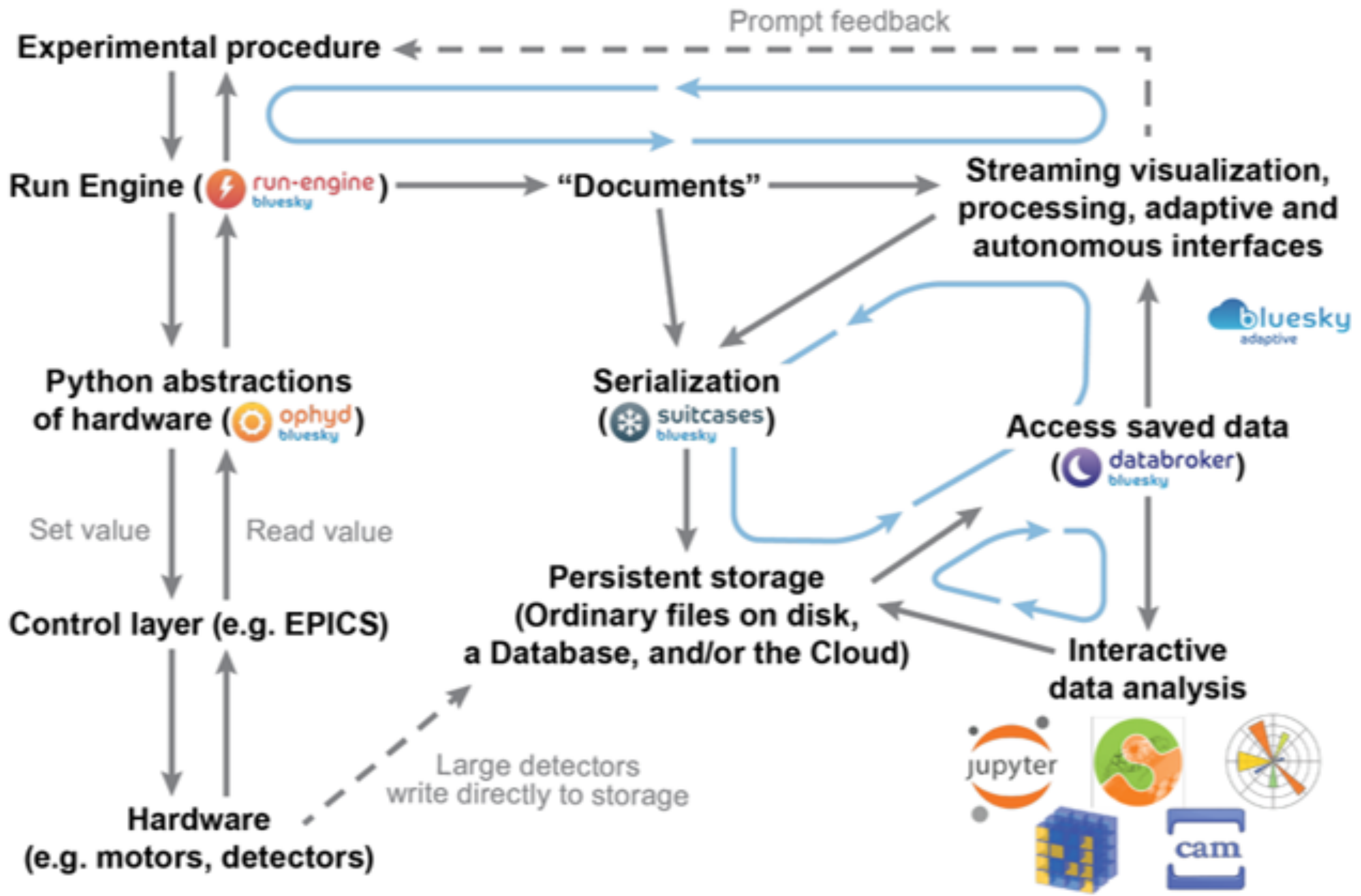


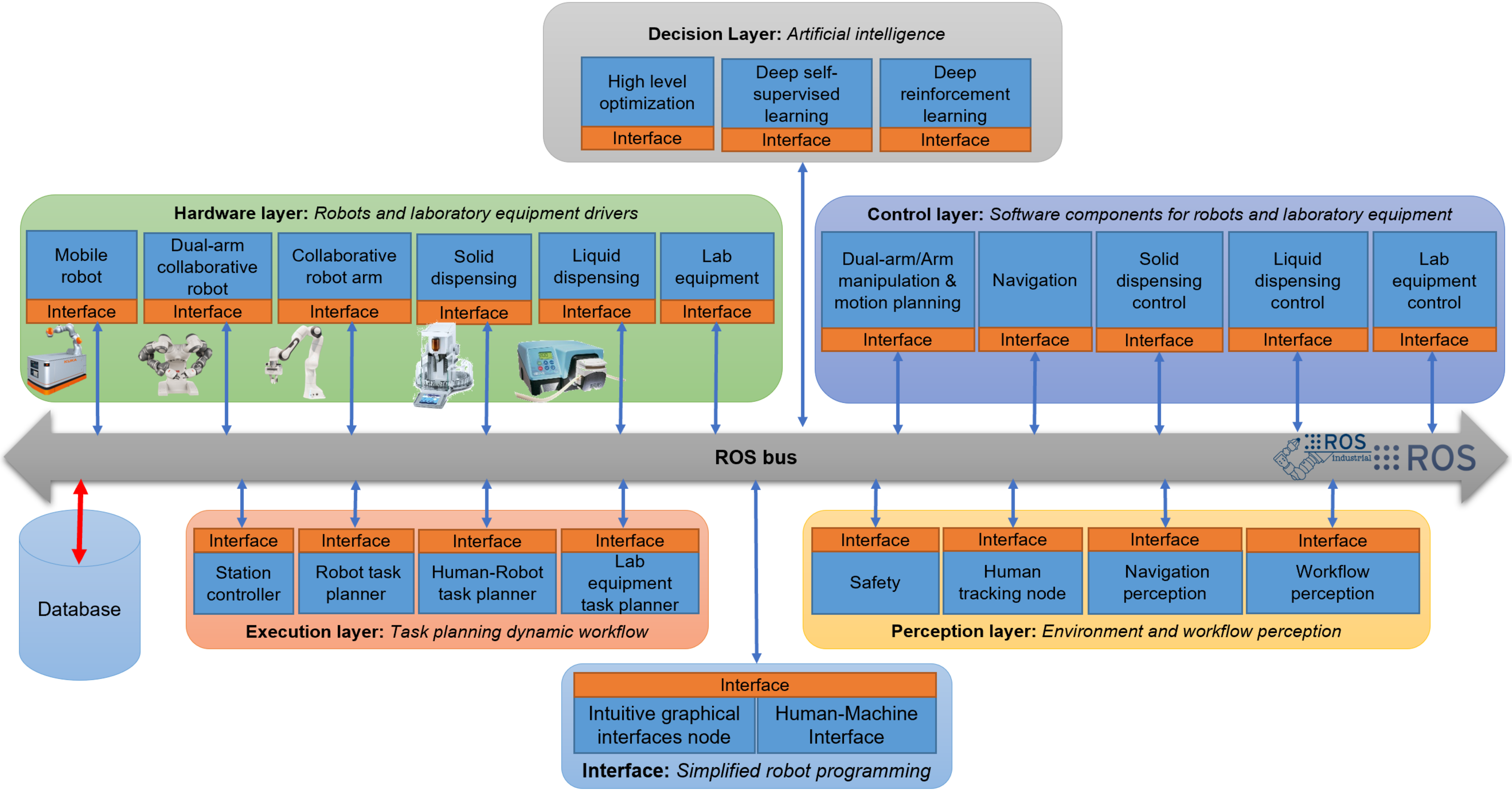


Mach. Learn.: Sci. Technol. **2**, 025025 (2021)

Artificial intelligence for beamline science



ROS-Laboratory



Diverse laboratory tasks connected via message bus, with real time bus for robotics.

Sample Preparation

Solid Dispensing:
/Dosing_status
/Door_position
/Sampler_position
/Dosing_target

Liquid Dispensing:
/Pump_status
/Pump_speed
/Pump_direction
/Timer

Mixing:
/mixer_status
/Speed_target
/Timer

Analysis

KUKA

ROS industrial

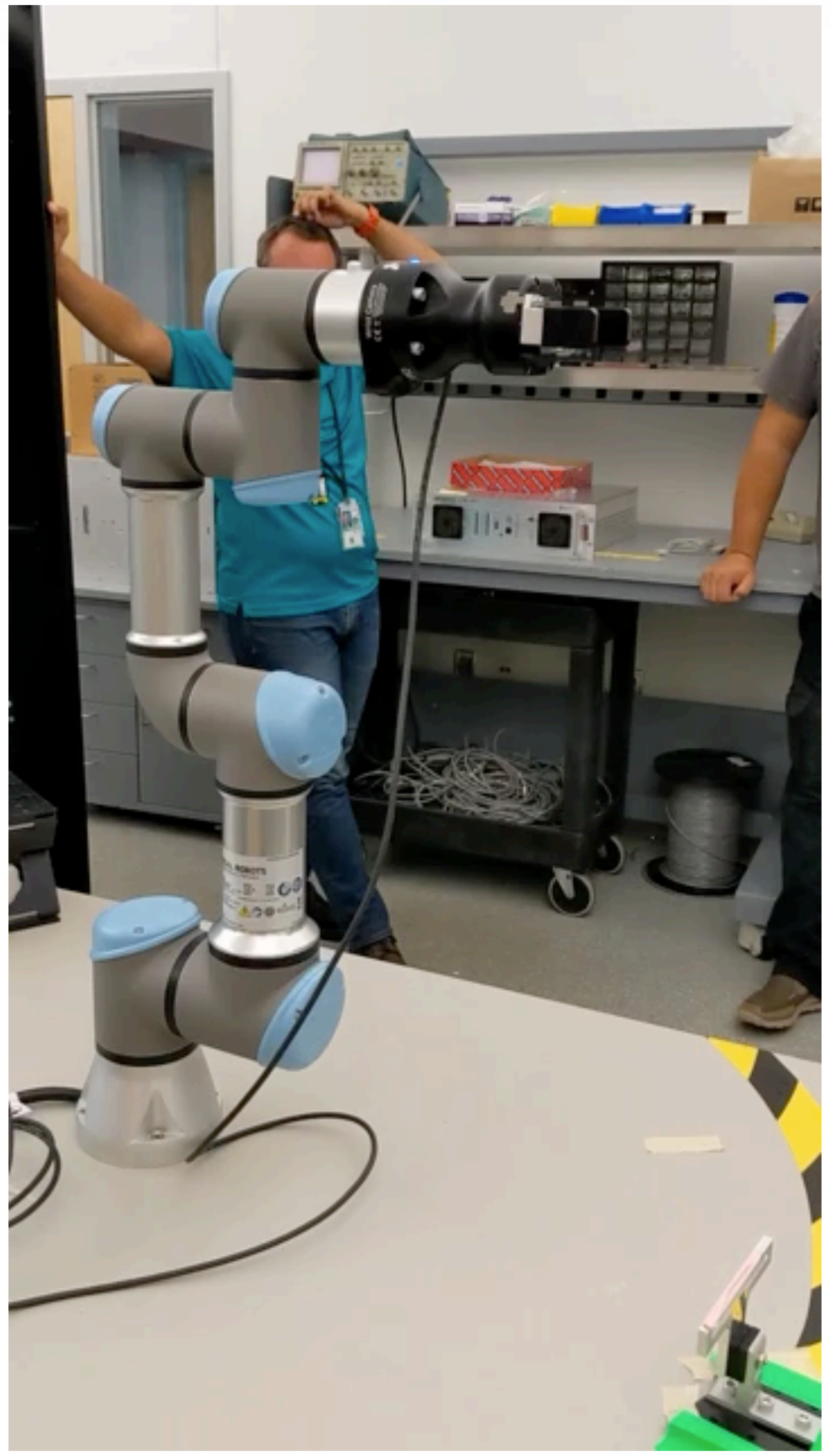
abb_driver

ROS industrial

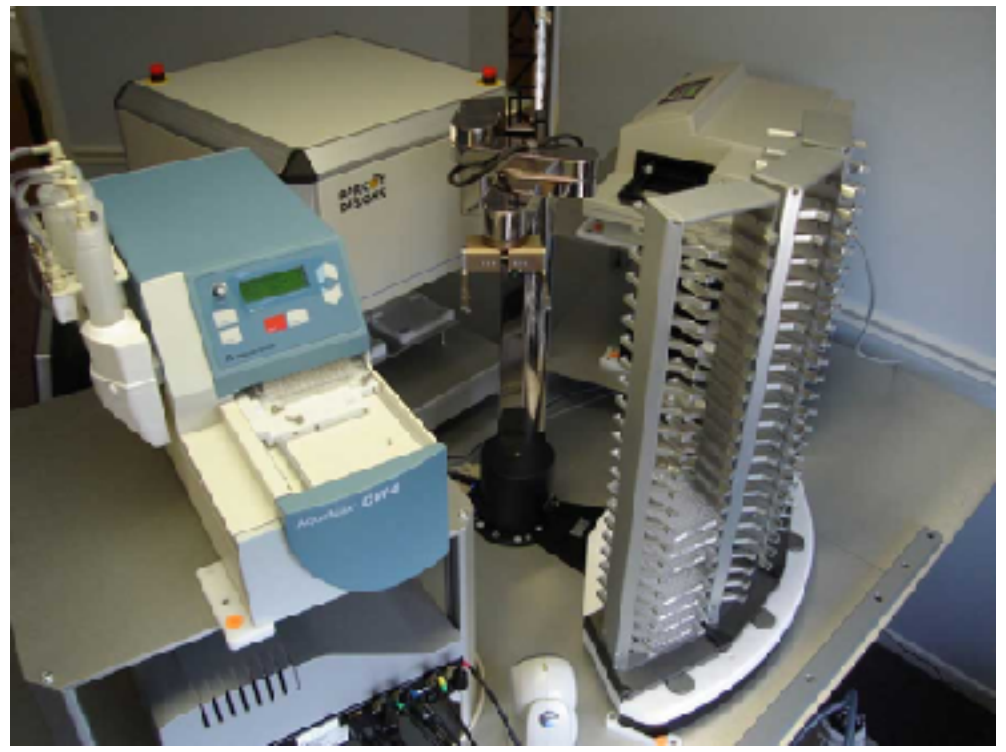
Mettler-Toledo
QS30 Autosampler

Watson Marlow
323DU Pump

IKA
ULTRA-TURRAX



Workcells are efficient self-contained unit operations.



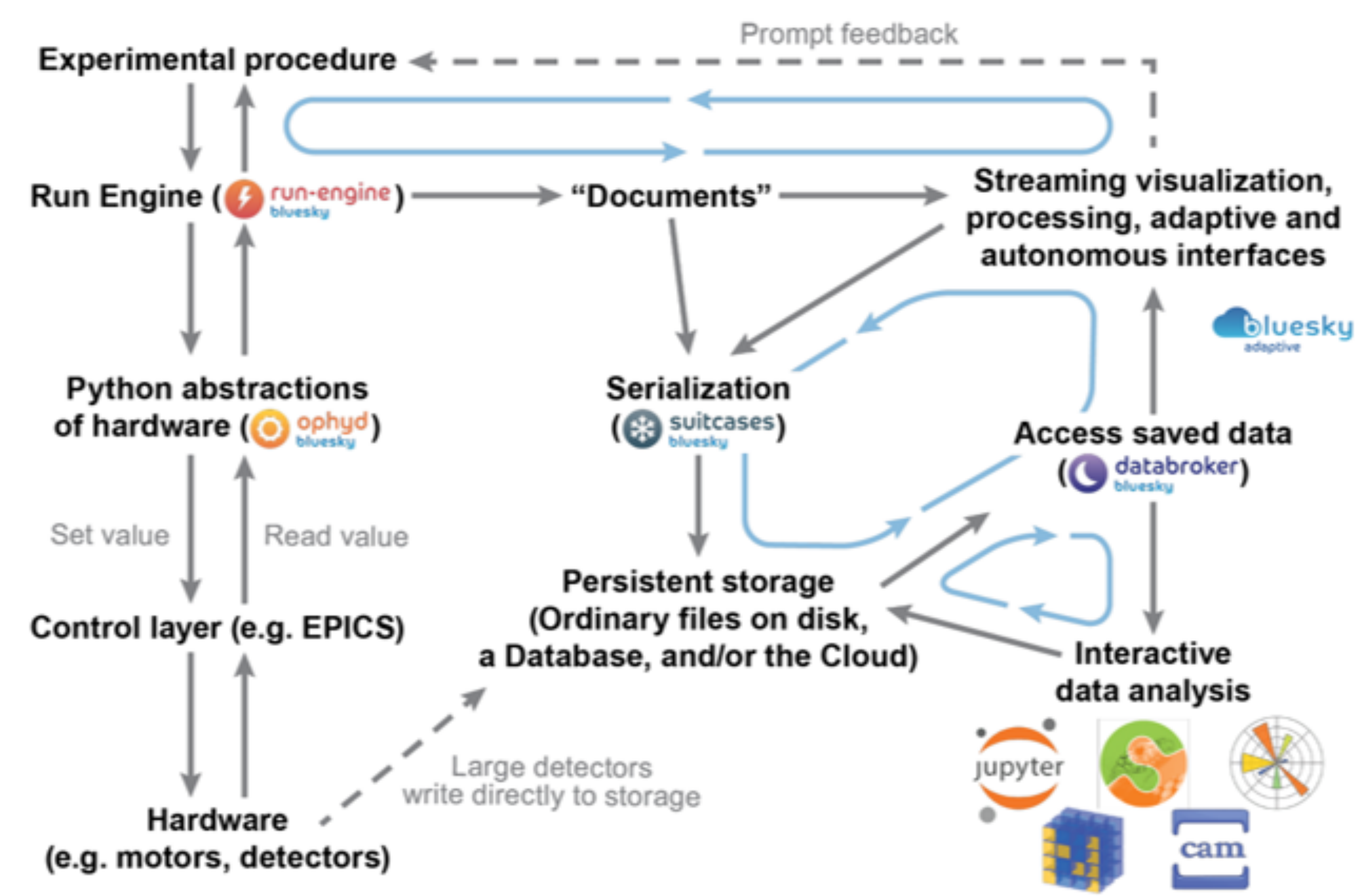
Automated Pipetting | Limited-function robot | Heavy robots (some integration) | Integrated Workcell

BigHat
BIOSCIENCES

Acknowledgements

Thank You!

- Using the right tool for the right job.
- Scalable infrastructure for linking models to experiments.
- Keeping the human in the loop.
- Open source automation is the frontier for autonomous experiments.



GitHub /Maffettone

@PhilMaffettone