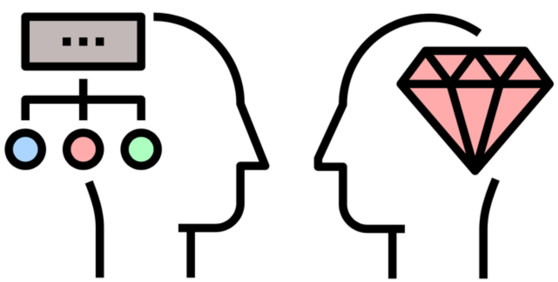
IMPERIAL
Department of Materials

Machine Learning for Materials

8. Accelerated Discovery



Aron Walsh

Department of Materials
Centre for Processable Electronics

Module Contents

“A *problem* in artificial intelligence is one which is so complex that it cannot be solved using any normal algorithm”

Hugh M. Cartwright, Applications of AI in Chemistry (1993)

Class Outline

Accelerated Discovery

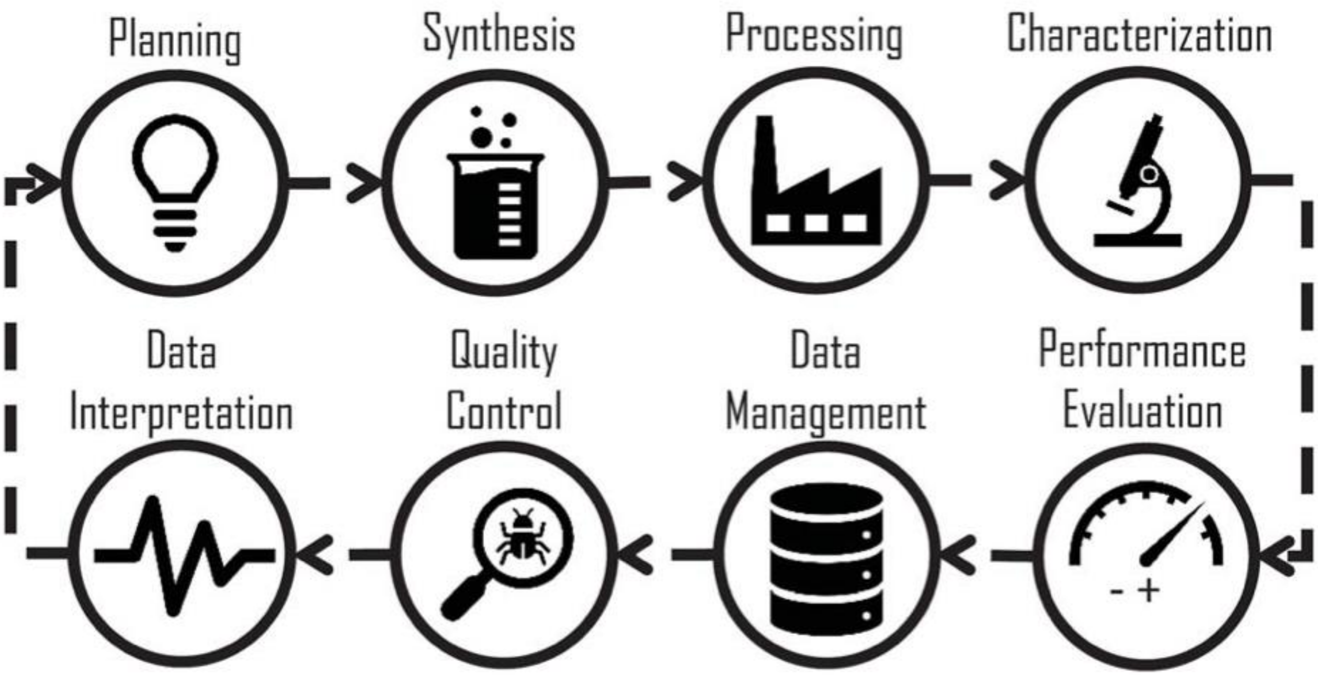
A. Automated Experiments

B. Bayesian Optimisation

C. Reinforcement Learning

Accelerate Scientific Discovery

Research can be broken down into a set of tasks that can each benefit from acceleration



Traditional research workflow

H. S. Stein and J. M. Gregoire, Chem. Sci. 10, 9640 (2019)

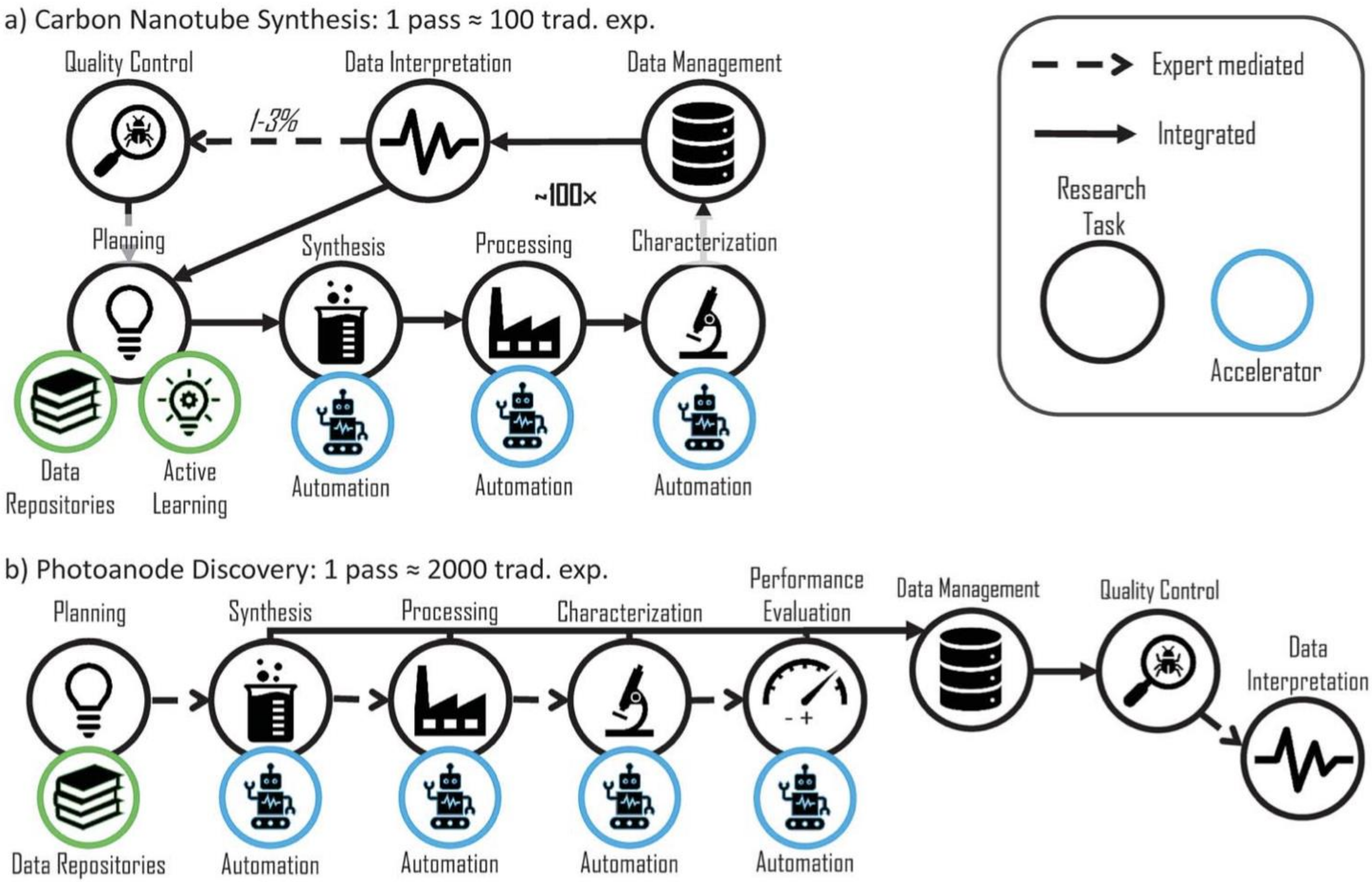
Accelerate Scientific Discovery

Research can be broken down into a set of tasks that can each benefit from acceleration

H. S. Stein and J. M. Gregoire, Chem. Sci. 10, 9640 (2019)

Accelerate Scientific Discovery

Workflow classification of published studies



H. S. Stein and J. M. Gregoire, Chem. Sci. 10, 9640 (2019)

Automation and Robotics

Execution of physical tasks to achieve a target using autonomous or collaborative robots

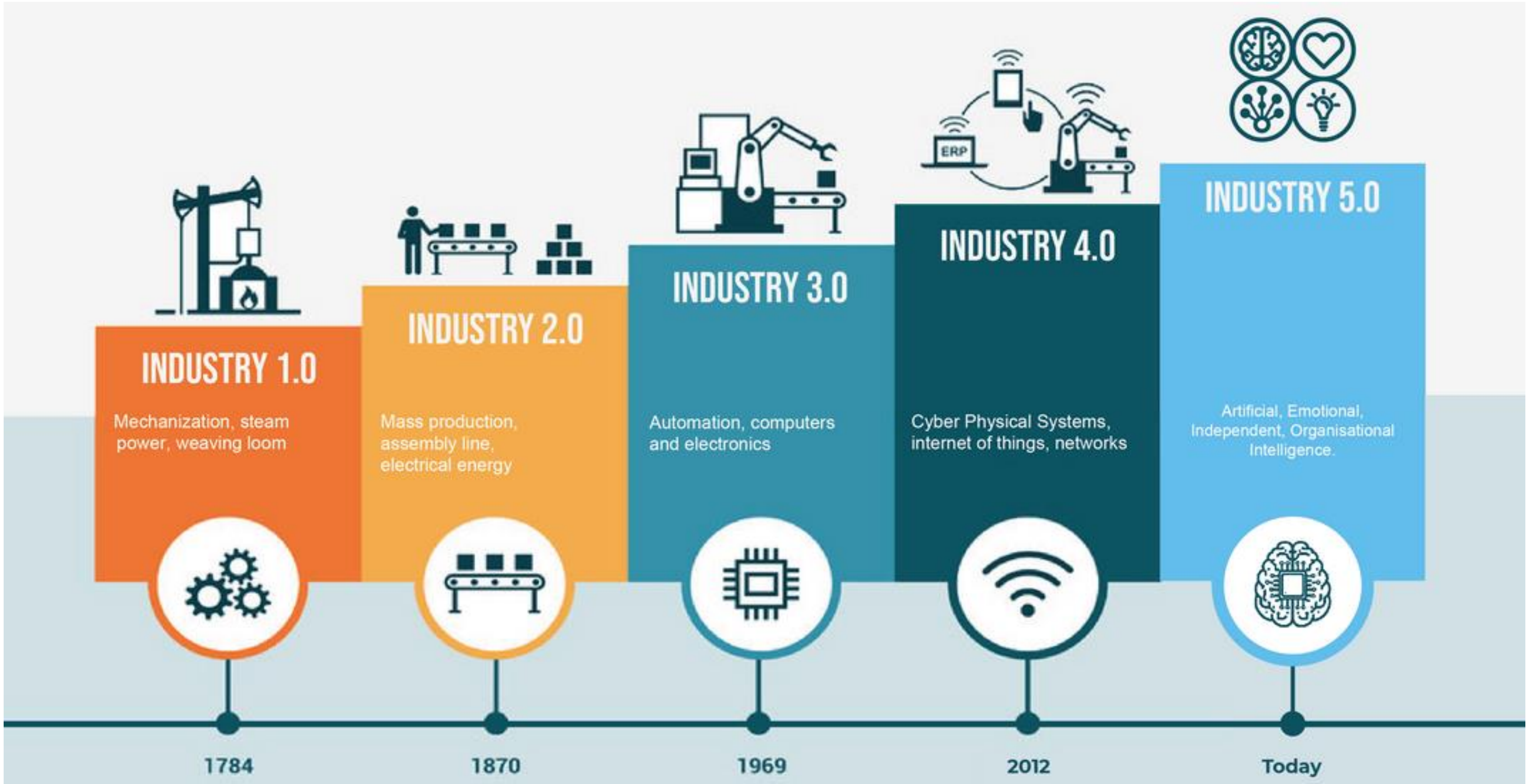
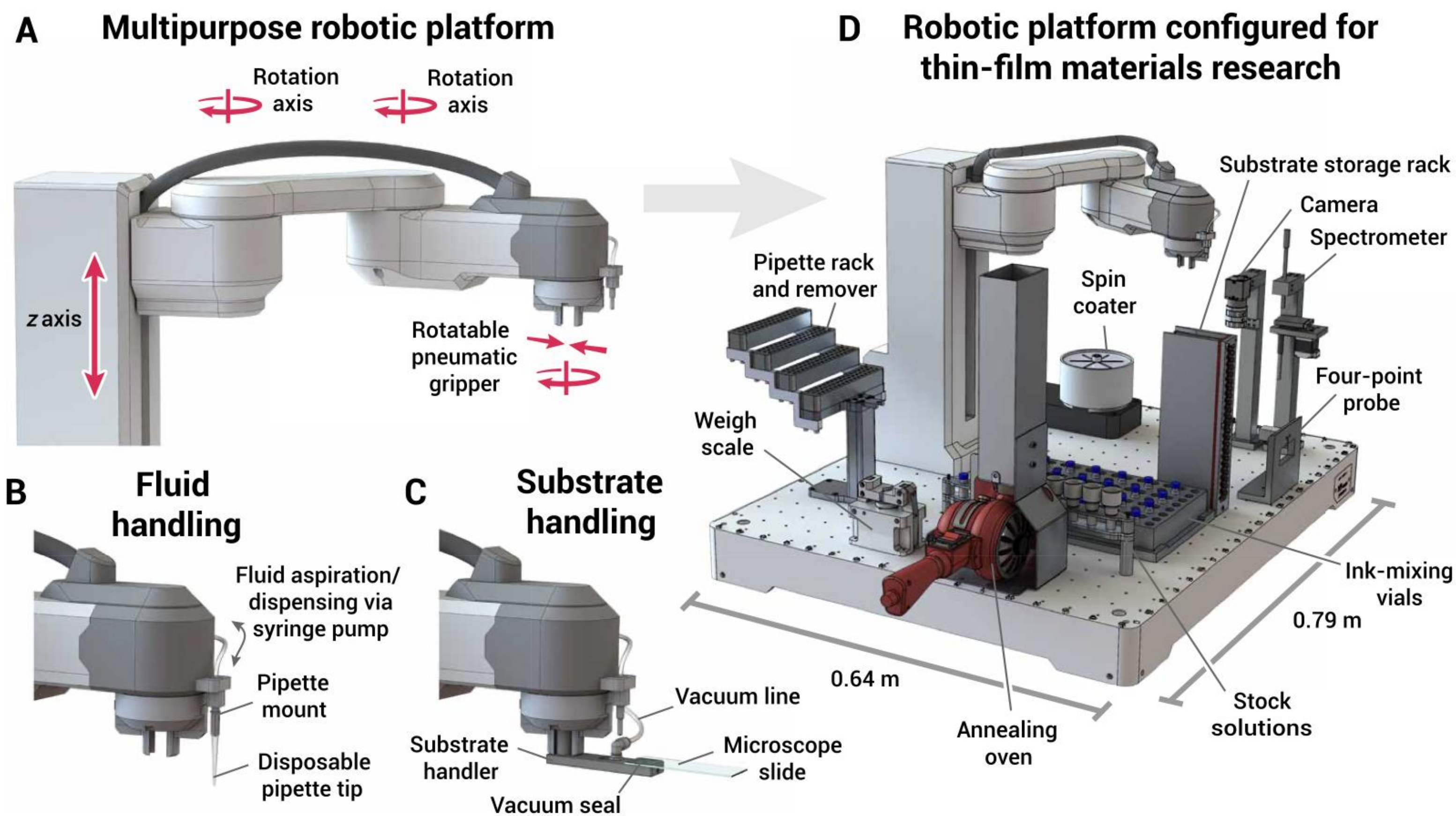


Image: https://www.thefifthindustrialrevolution.co.uk

Automation and Robotics

Robots can be tailored for a wide range of materials synthesis and characterisation tasks



B. P. MacLeod et al, Science Advances 6, eaaz8867 (2020)

Automation and Robotics

Self-driving labs (SDL) are now operating

N. J. Szymanski et al, Nature 624, 86 (2023); Phys. Rev. Energy 3, 011002 (2024)

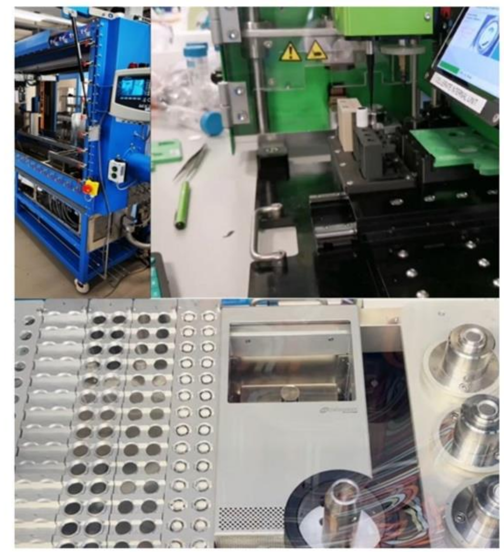
Flexible Automation Systems

Modular hardware with computer-controlled synthesis and characterisation

ROAR CENTRE FOR RAPID ONLINE ANALYSIS OF REACTIONS

ATLAS AUTOMATED HIGH-THROUGHPUT PLATFORM SUITE

DIGIBAT Automated Energy Research



Small Molecules

Materials

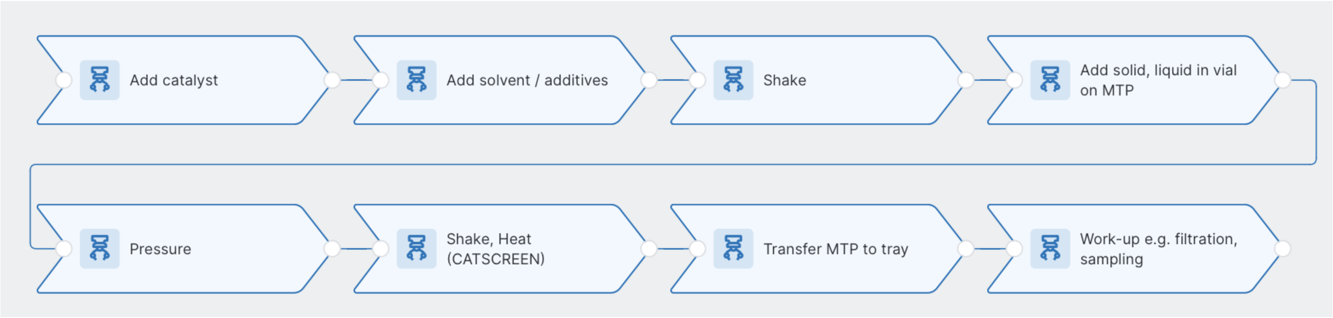
Applications

DIGIBAT: In collaboration with Magda Titirici, Ifan Stephens, and others (ICL)

Flexible Automation Systems

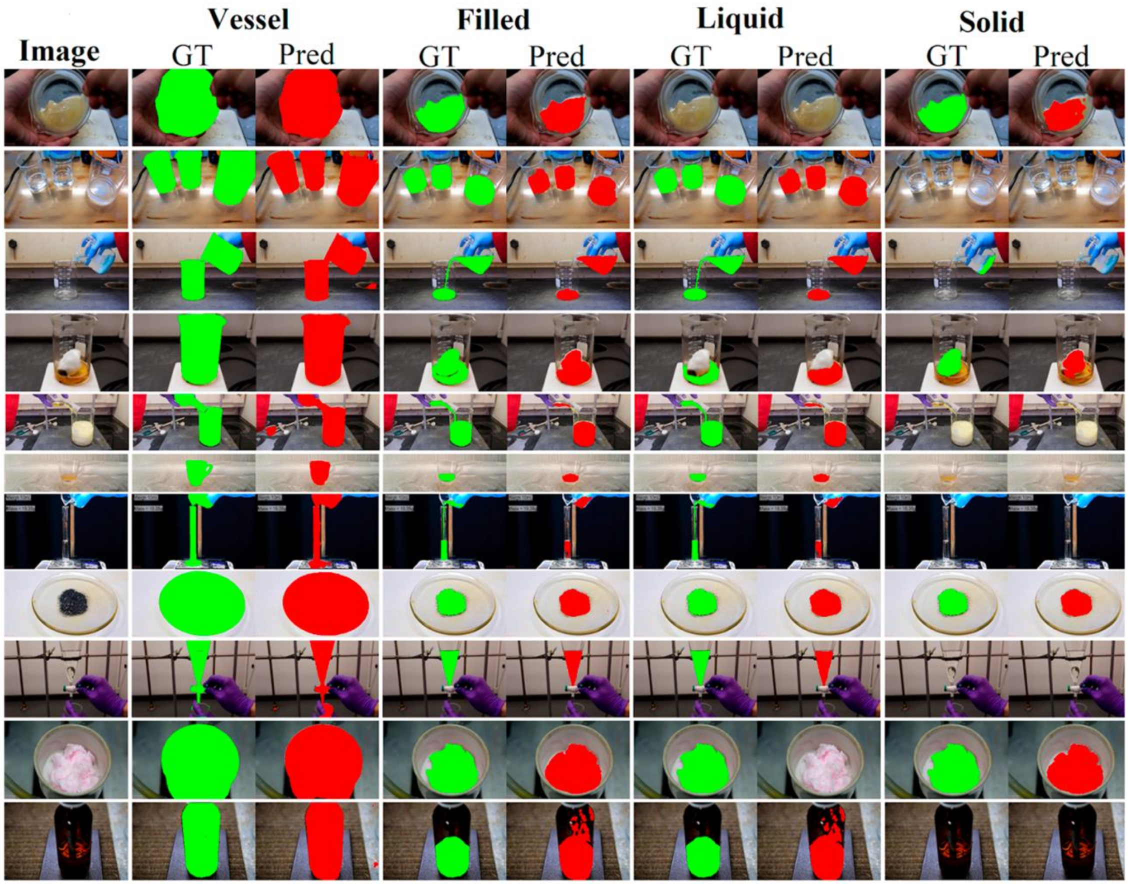
Automation platforms designed to deliver complex research workflows (fixed platform or mobile)

Usually a mix of proprietary code, with GUI and Python API for user control



Automation and Robotics

Robots can be equipped with sensors and artificial intelligence to interact with their environment



Adapting computer vision models for laboratory settings

GT = ground truth
Pred = predicted

S. Eppel et al, ACS Central Science 6, 1743 (2020)

Automation and Robotics

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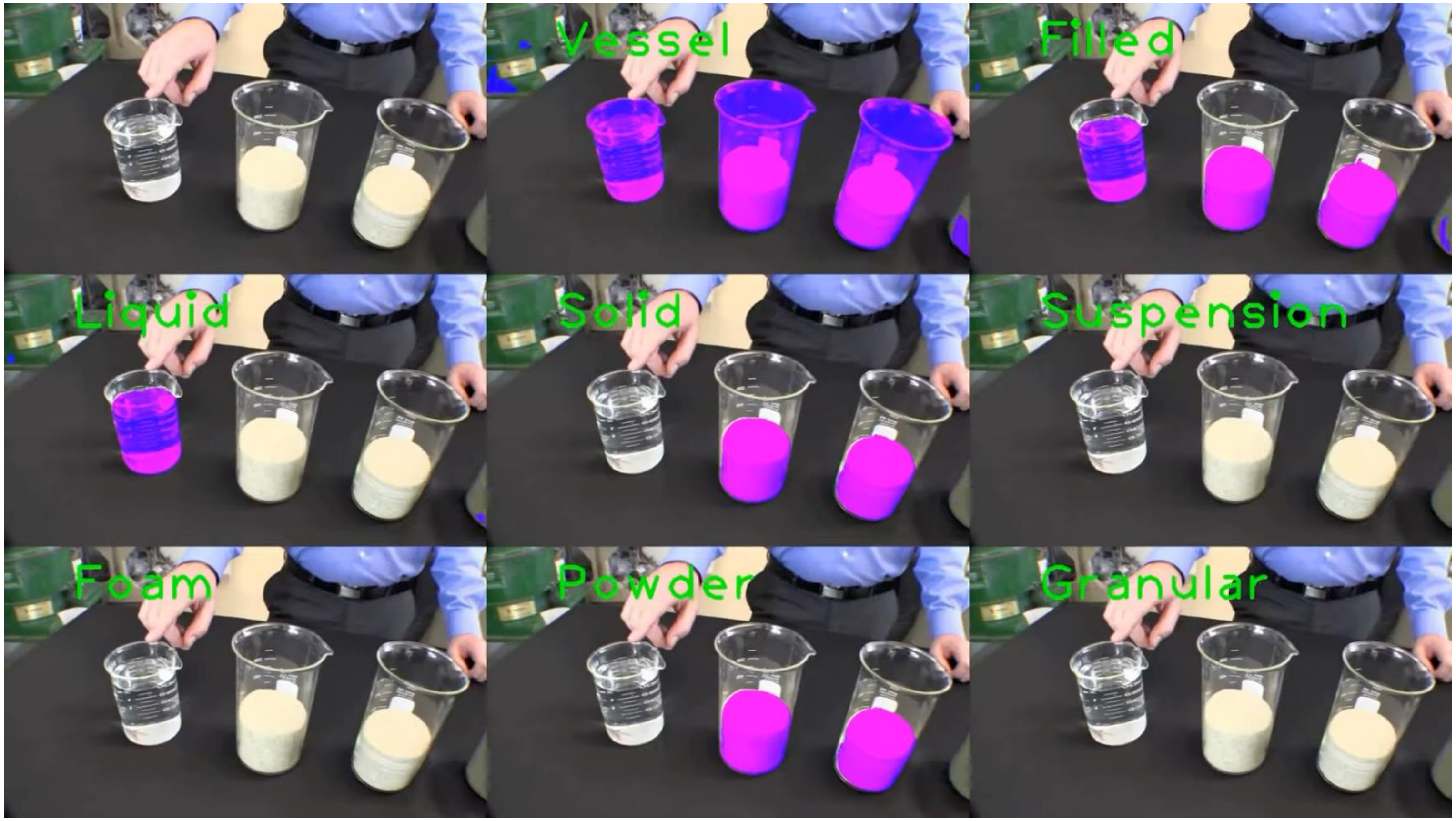


https://www.youtube.com/watch?v=K7I2QJcIyBQ

Optimisation

Algorithms to efficiently achieve a desired research objective. Considerations:

Objective function (O): Materials properties or device performance criteria, e.g. battery lifetime

Parameter selection: Variables that can be controlled, e.g. temperature, pressure, composition

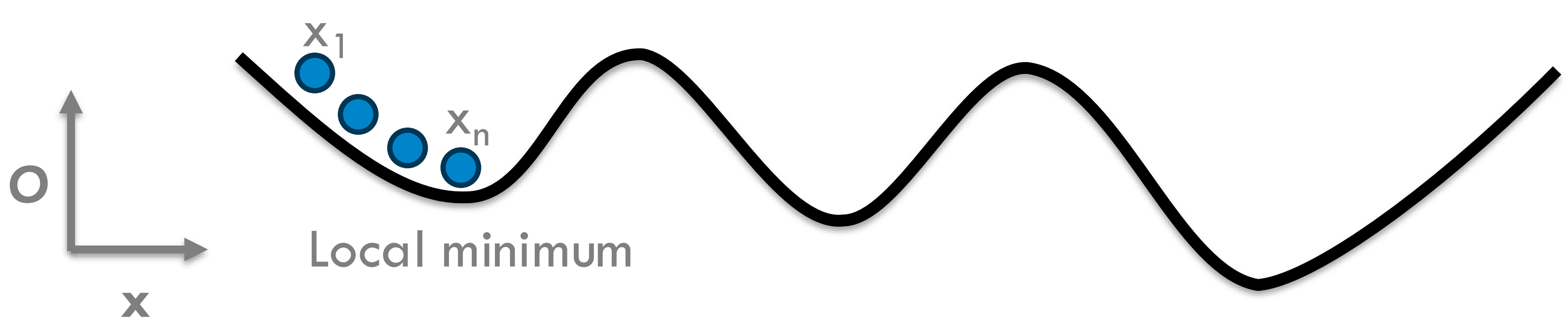
Data acquisition: How the data is collected, e.g. instruments, measurements, automation

Optimisation Algorithms

Local optimisation – find the best solution in a limited region of the parameter space (**x**)

Gradient based: iterate in the direction of the steepest gradient ($d\mathbf{O}/d\mathbf{x}$), e.g. gradient descent

Hessian based: use information from the second derivatives ($d^2\mathbf{O}/d\mathbf{x}^2$), e.g. quasi-Newton



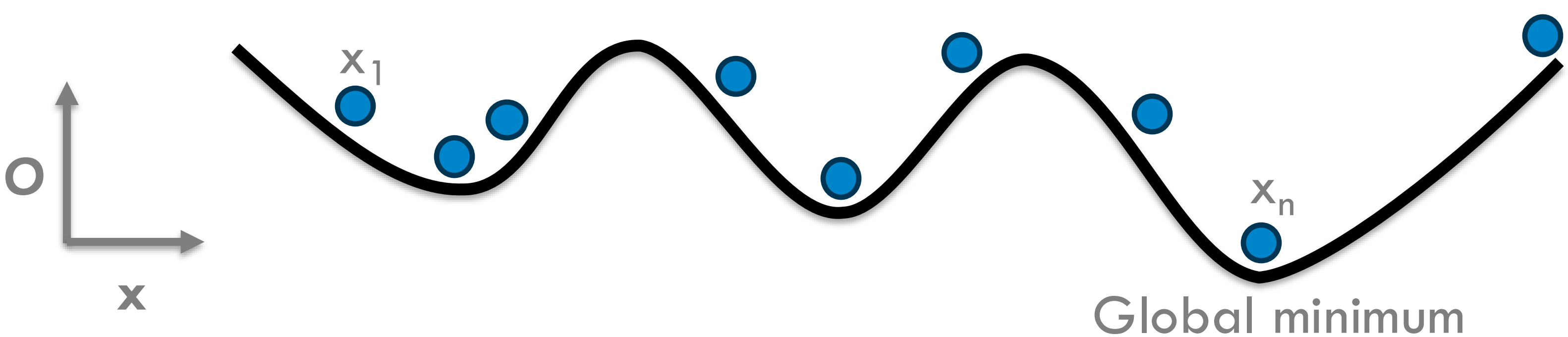
The same concepts are involved in ML model training

Optimisation Algorithms

Global optimisation – find the best solution from across the entire parameter space

Numerical: iterative techniques to explore parameter space, e.g. downhill simplex, simulated annealing

Probabilistic: incorporate probability distributions, e.g. Markov chain Monte Carlo, Bayesian optimisation



The same concepts are involved in ML model training

Class Outline

Accelerated Discovery

A. Automated Experiments

B. Bayesian Optimisation

C. Reinforcement Learning

Bayesian Optimisation (BO)

Use prior (measured or simulated) data to decide which experiment to perform next

(parameters to sample)

Probabilistic (Surrogate) Model

Approximation of the true objective function

O(**x**) ~ f(**x**), e.g. Gaussian process, GP(x,x')

new known

Acquisition Function

Selection of the next sample point, e.g. upper confidence bound (UCB), probability of improvement (PI), expected improvement (EI)

J. Močkus, Optimisation Techniques 1, 400 (1974)

Bayesian Optimisation (BO)

Use prior (measured or simulated) data to decide which experiment to perform next

(parameters to sample)

Probabilistic (Surrogate) Model

Gaussian process: $f(x) \sim GP(\mu(x), k(x,x'))$

mean function

Gaussian kernel function

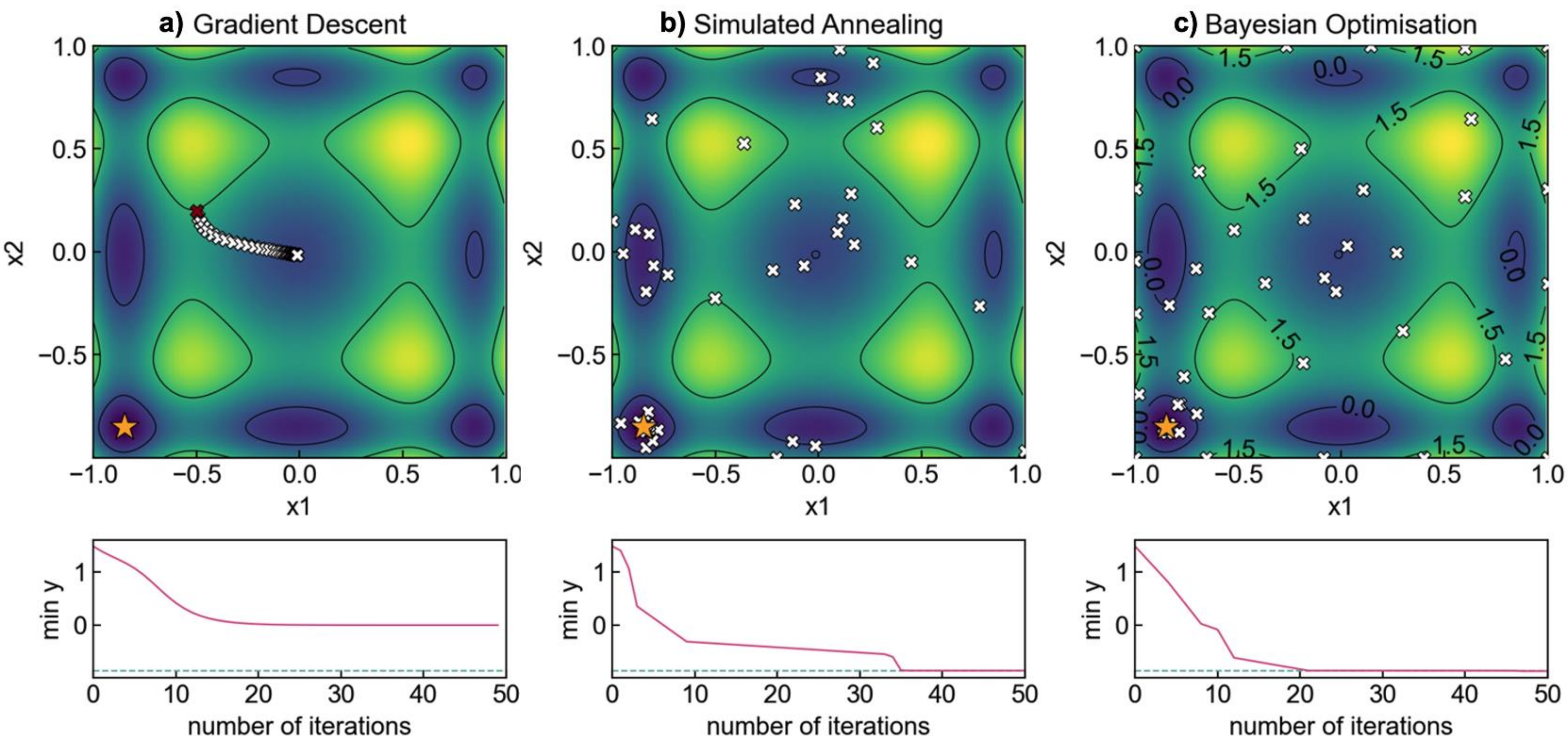
$k(x,x')$ measures the similarity between points x and x'

- Kernel controls function smoothness and defines uncertainty
  - Unobserved point x influenced by similar prior data
- Dissimilar points default to the mean with high uncertainty

J. Močkus, Optimisation Techniques 1, 400 (1974)

Bayesian Optimisation (BO)

Use prior (measured or simulated) data to decide which <u>experiment to perform</u> next



Bayesian optimisation for chemistry: Y. Wu et al, Digital Disc. 3, 1086 (2024)

Exploration–Exploitation Tradeoff

Upper confidence bound selects points that maximise the predicted function value of the model

$$x_{next} = \max_{x}\left(\mu(x) + \beta\sigma(x) \right)$$

What to do next

Prediction based on prior knowledge

Weighted Uncertainty

A tunable hyperparameter of UCB

$\beta < 1$ focus on exploitation

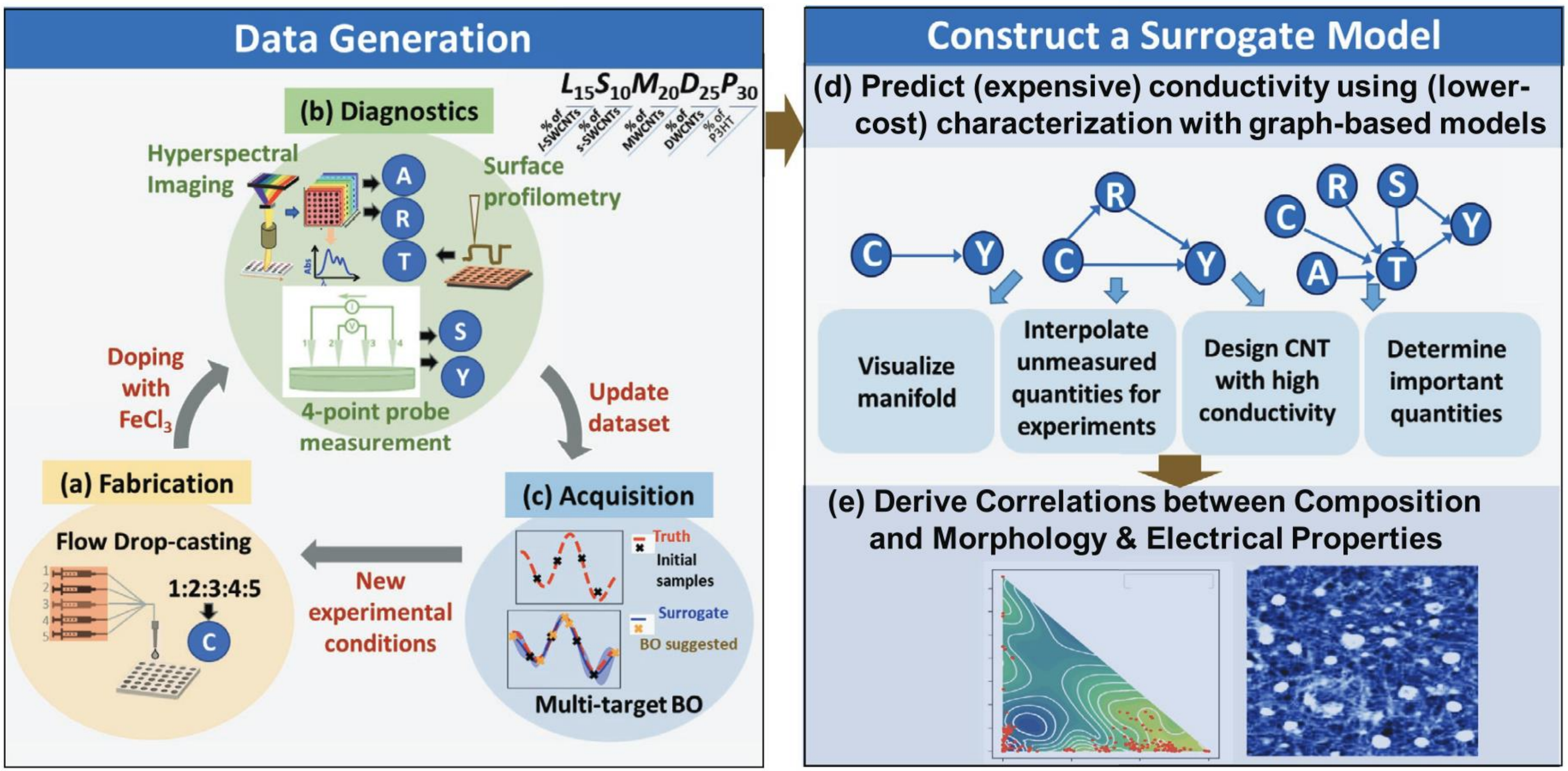
$\beta \sim 1$ balance risk and reward

$\beta > 1$ focus on exploration

N. Srinivas et al, IEEE Transactions on Information Theory, 58 (2012)

Applications of BO

Application to maximise electrical conductivity of a composite (P3HT-CNT) thin-film



D. Bash et al, Adv. Funct. Mater. 31, 2102606 (2021)

Applications of BO

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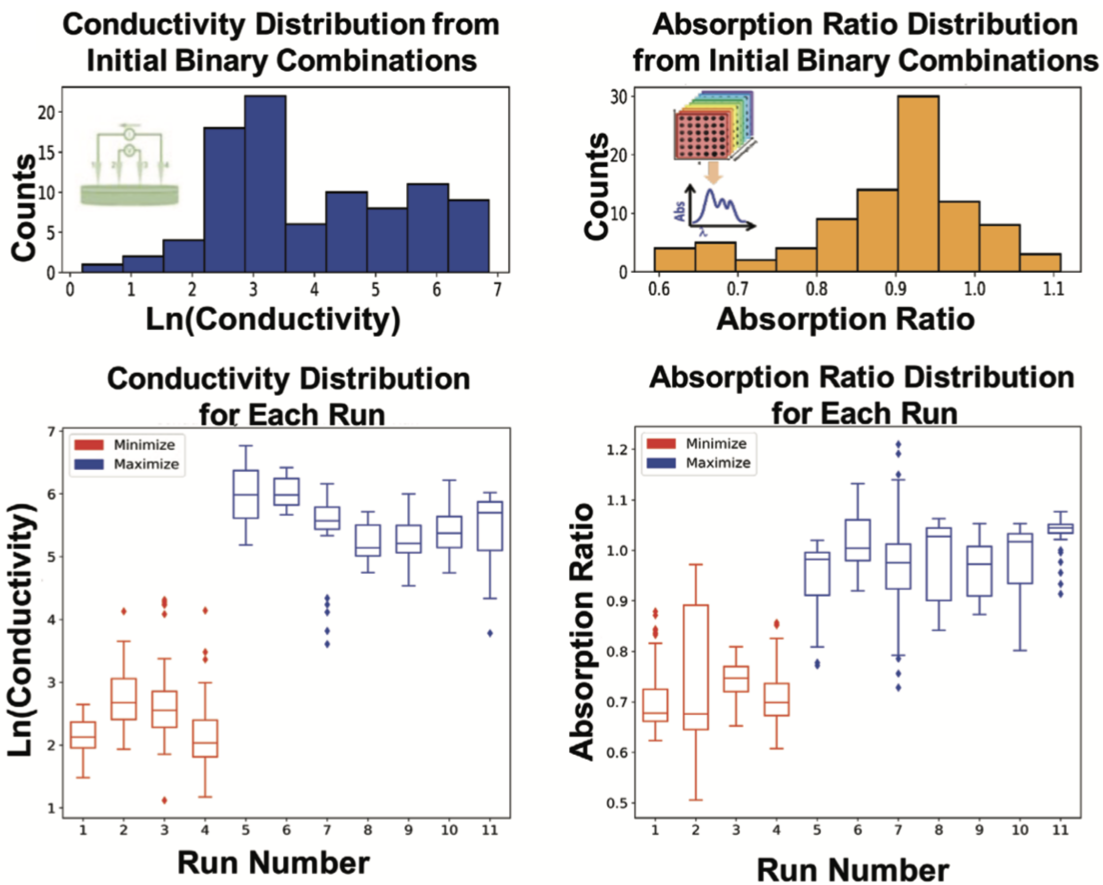


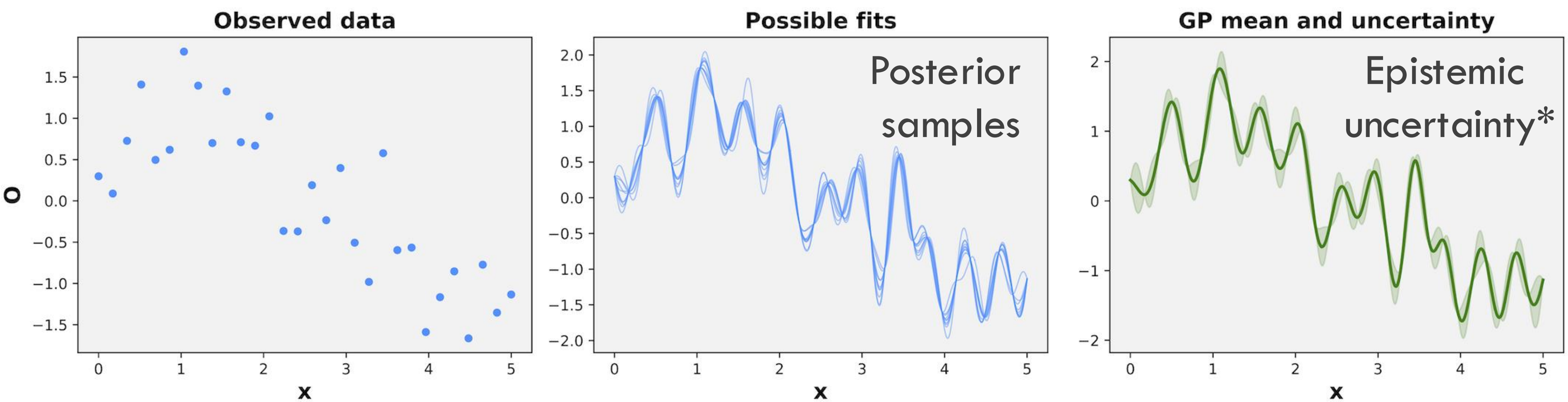
D. Bash et al, Adv. Funct. Mater. 31, 2102606 (2021)

Active Learning (AL)

BO: find inputs that maximise the objective function

AL: find inputs that enhance model performance

Target unknown regions with the largest uncertainty

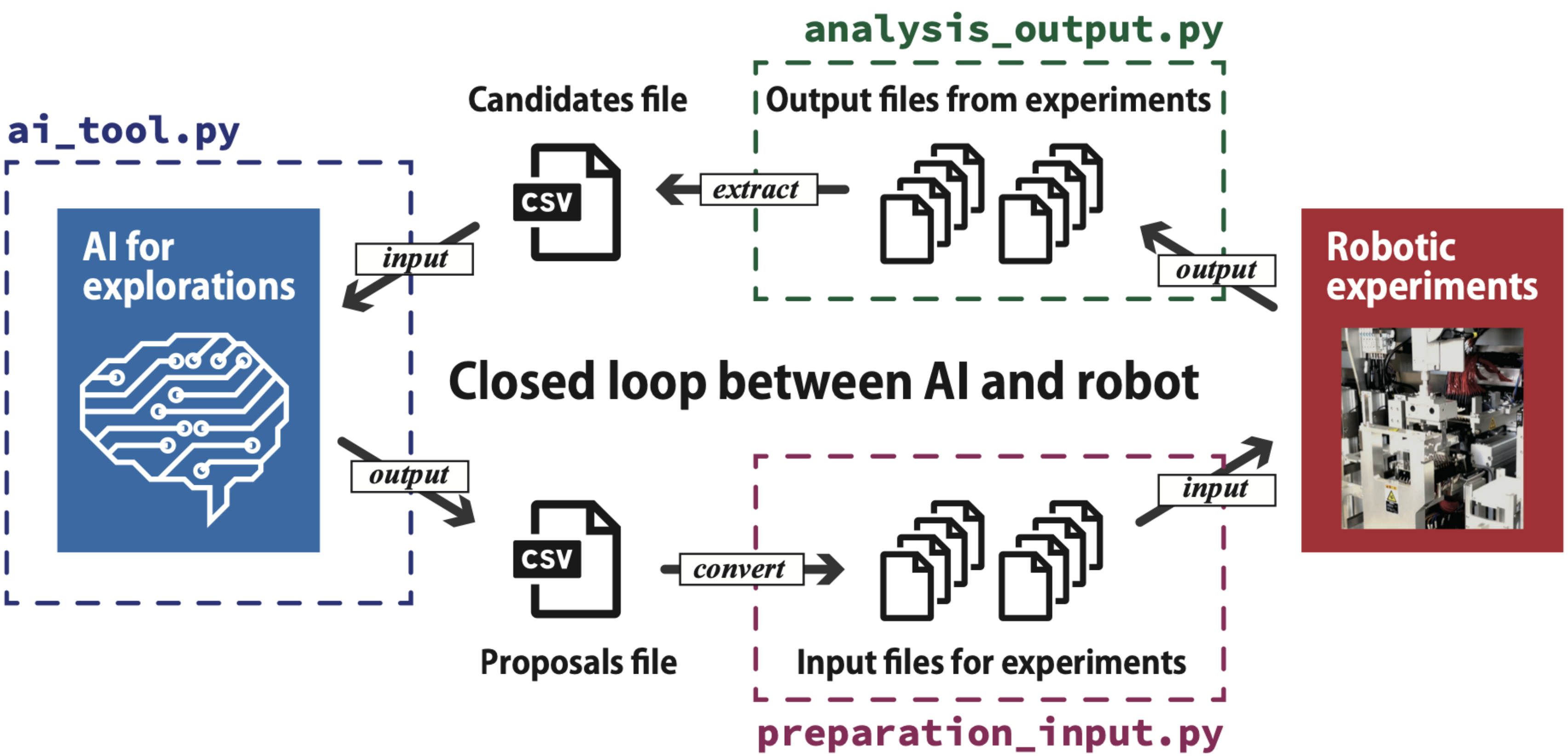


The Gaussian process is updated with new observations to yield revised function values and uncertainty

* Reducible uncertainty associated with lack of information

Integrated Research Workflows

Feedback loop between optimisation model and automated experiments



NIMS-OS: R. Tamura, K. Tsuda, S. Matsuda, arXiv:2304.13927 (2023)

Integrated Research Workflows

Feedback loop between optimisation model and automated experiments

Initial stage of the candidates file

descriptor 1	...	descriptor d	objective 1	...	objective l
1	...	0			
1	...	0.5			
1	...	1			
0.5	...	0			
0.5	...	0.5			
0.5	...	1			
0	...	0			
0	...	0.5			
0	...	1			

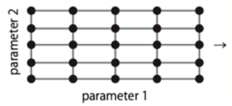
After three experiments

Candidates file after some experiments

descriptor 1	...	descriptor d	objective 1	...	objective l
1	...	0			
1	...	0.5	12	...	20
1	...	1			
0.5	...	0			
0.5	...	0.5			
0.5	...	1	5	...	8
0	...	0			
0	...	0.5			
0	...	1	23	...	2

Examples for the list of descriptors

Discretized parameter space



parameter1	parameter2
0	0
0	0.1
0	0.2
:	:

Combination of materials

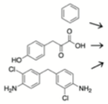
	A	B	C	D	E	F	...
ABC →	1	1	1	0	0	0	...
BDF →	0	1	0	1	0	1	...
CEF →	0	0	1	0	1	1	...
	:	:	:	:	:	:	...

Materials descriptors

	Number	MendeleevNumber	Atomic Weight	MeltingT	Column	Row	
$Fe_{0.3}Ni_{0.2}Mn_{0.2}$ →	26.28	55.85	56.39	1703.85	8.28	4.0	...
$Ag_{0.8}Cd_{0.2}$ →	47.2	66.0	108.77	1106.78	11.20	5.0	...
$Hf_{0.5}Ta_{0.5}$ →	72.5	46.5	179.71	2898.0	4.5	6.0	...
	:	:	:	:	:	:	...

e.g. by magpie

Fingerprint of molecules



16	50	80	389	1088	1313	...
0	0	0	1	1	0	...
1	0	1	1	0	1	...
0	1	1	0	0	0	...
:	:	:	:	:	:	...

e.g. by Morgan fingerprint

NIMS-OS: R. Tamura, K. Tsuda, S. Matsuda, arXiv:2304.13927 (2023)

Class Outline

Accelerated Discovery

A. Automated Experiments

B. Bayesian Optimisation

C. Reinforcement Learning

Reinforcement Learning (RL)

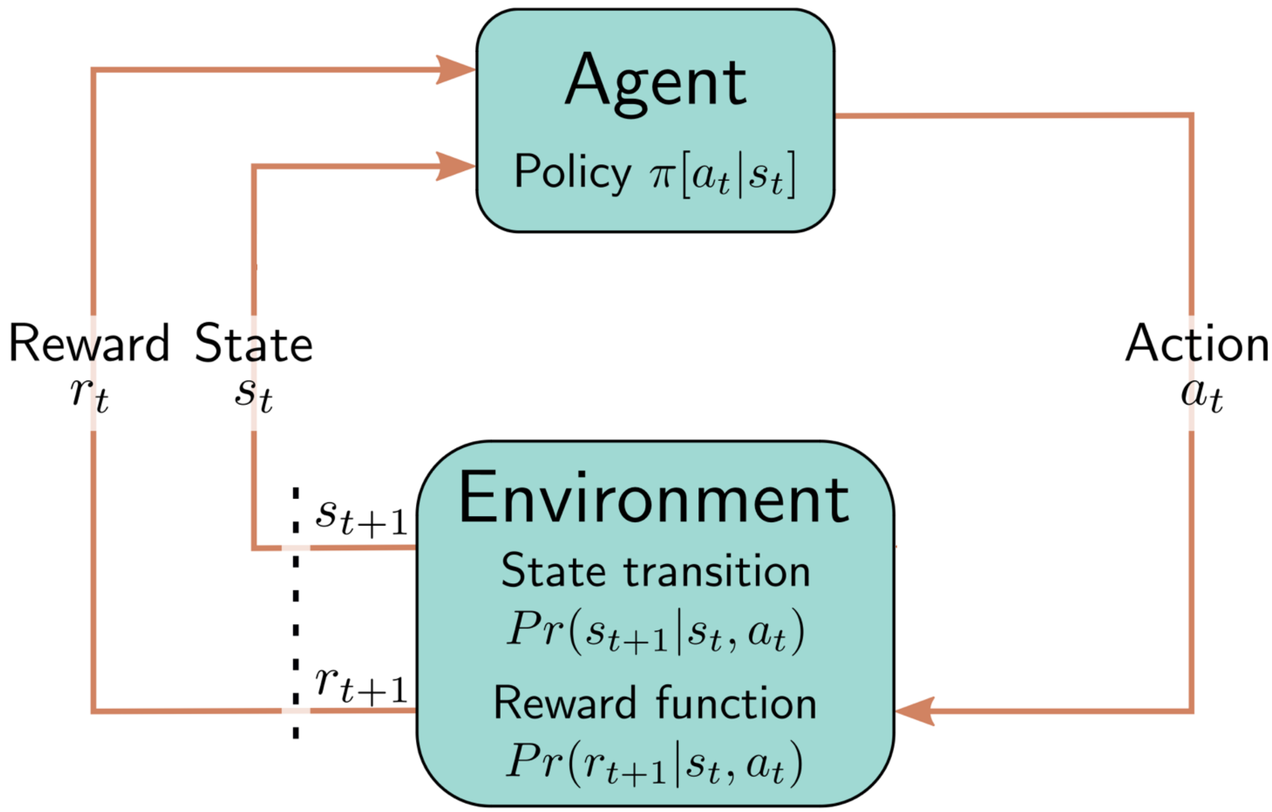
An agent interacts with an environment to learn decision-making strategies that achieve a specific goal

Nintendo


Boston robotics

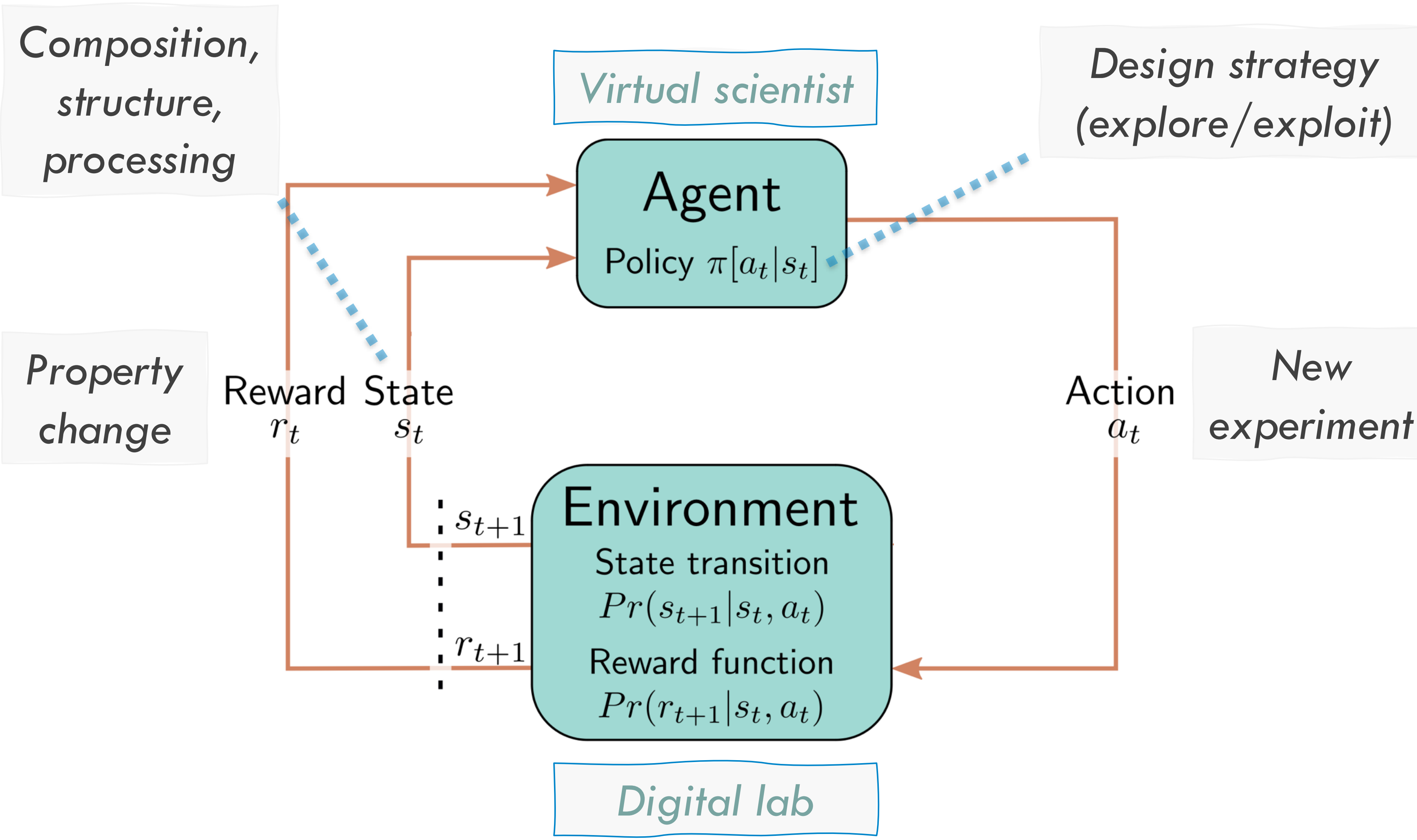
Early applications in video games (maximise score), finance (maximise profit), and robotics (perform a task)

Reinforcement Learning (RL)



RL schematic: S. J. D. Prince, https://udlbook.github.io

Reinforcement Learning (RL)



RL schematic: S. J. D. Prince, https://udlbook.github.io/udlbook

RL Policy

Data-driven decision making that adapts over time

Probability of action a_t given state s_t

Expected reward for action a_t

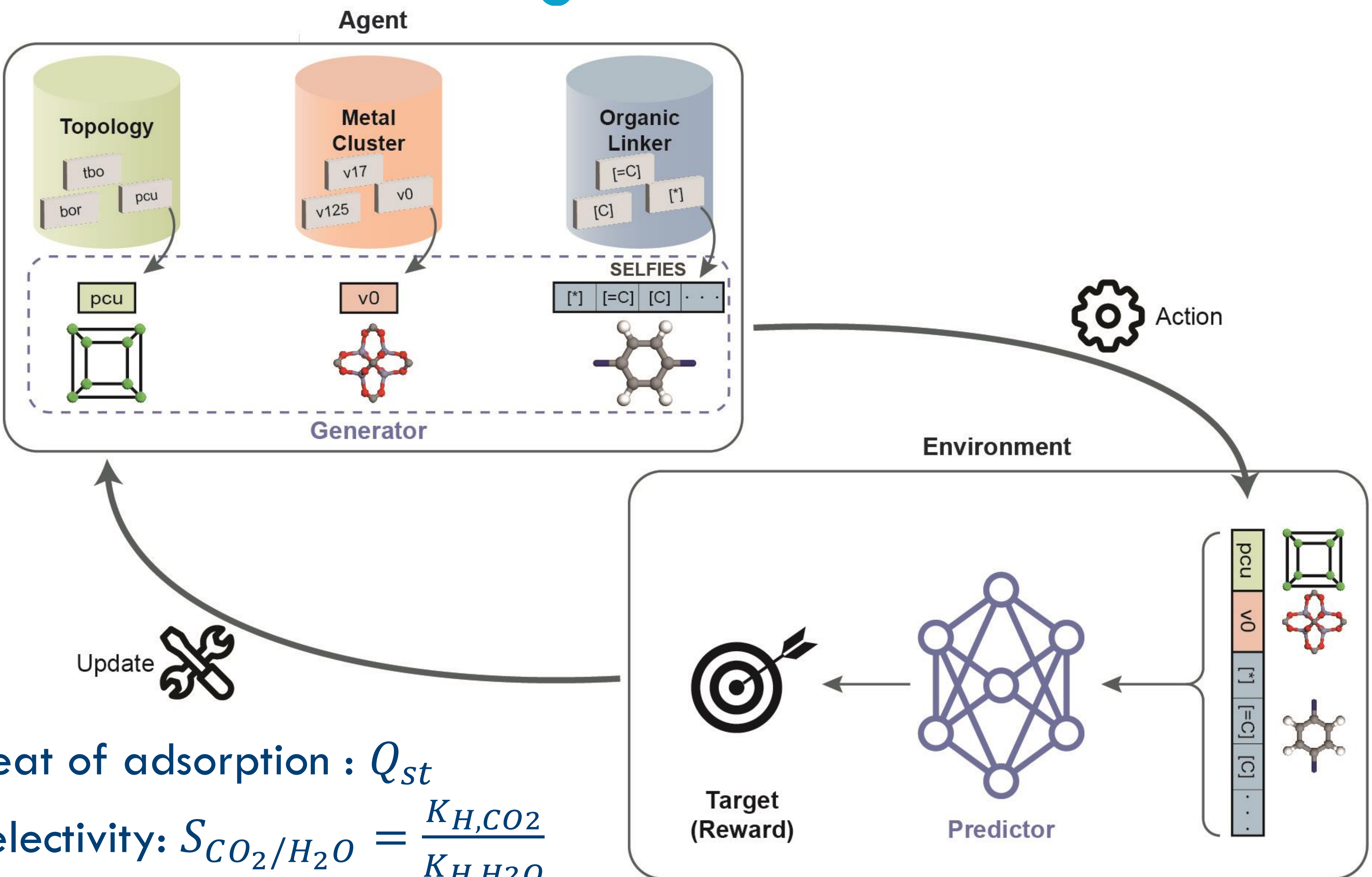
$$\pi(a_t|s_t) = \frac{\exp(Q(s_t, a_t)/\tau)}{\sum_{a' \in \mathcal{A}} \exp(Q(s_t, a')/\tau)}$$

Sum over all possible actions

Effective temperature for exploration/exploitation balance

This familiar equation is a softmax (Boltzmann) policy

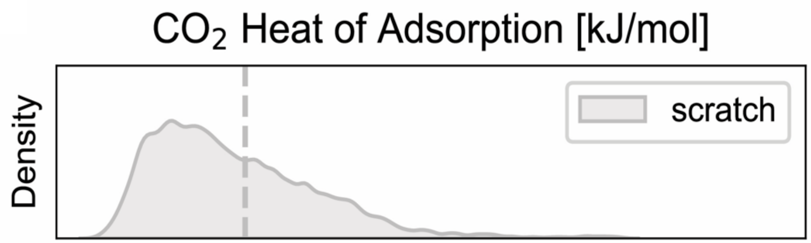
RL of Metal-Organic Frameworks

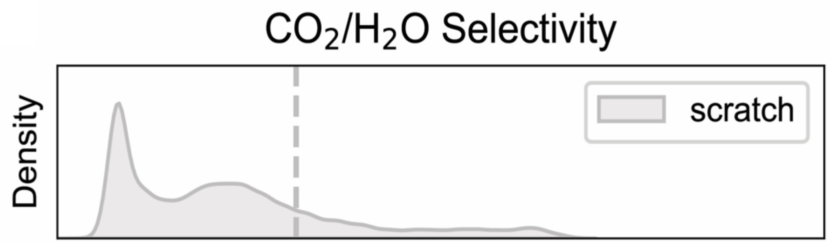


Heat of adsorption : Q_{st}

Selectivity: $S_{CO_2/H_2O} = \frac{K_{H,CO2}}{K_{H,H2O}}$

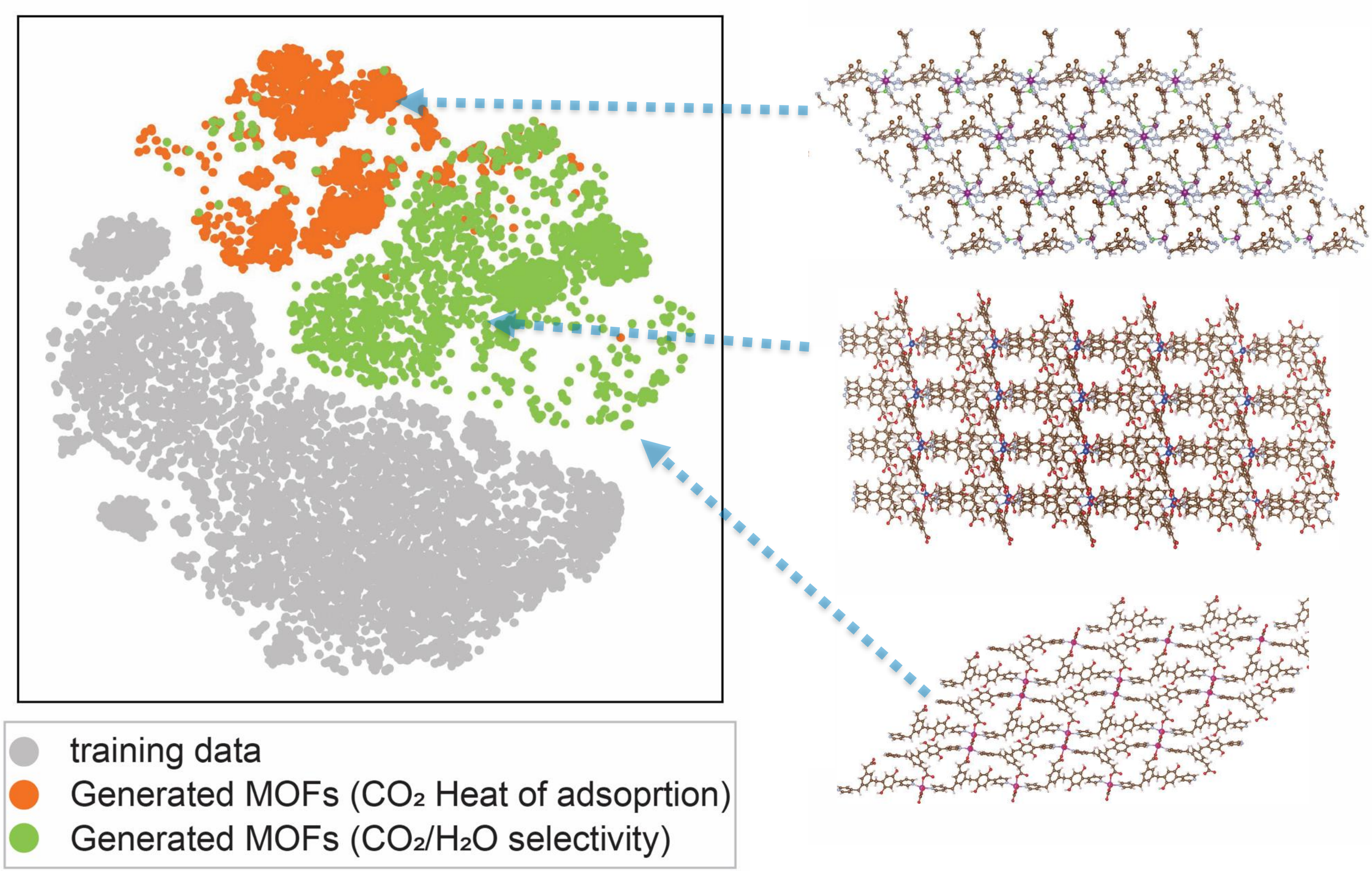
RL of Metal-Organic Frameworks





Hyunsoo Park et al, Digital Discovery 3, 728 (2024)

RL of Metal-Organic Frameworks



Hyunsoo Park et al, Digital Discovery 3, 728 (2024)

Optimisation Strategy

	Advantages	Disadvantages
Combinatorial (Enumeration)	- Exhaustive search ensures no possibilities are missed - Simple to implement and understand	- Inefficient for high-dimensional spaces - Maximises number of experiments and dataset
Bayesian Optimisation	- Efficiently exploit data - Works with noisy and expensive evaluations - Can use prior knowledge	- Performance depends on surrogate model & acquisition function - May struggle with high-dimensional spaces
Reinforcement Learning	- Learns optimal policies through interaction - Can handle dynamic and complex environments	- Requires large amounts of data for training - High computational cost - May converge slowly

Obstacles to Closed Loop Discovery

- **Materials complexity:** complex structures, compositions, processing sensitivity
- **Data quality and reliability:** errors and inconsistencies that waste resources
- **Cost of automation:** major investment required in infrastructure and training
- **Adaptability:** systems and workflows may be difficult to reconfigure for new problems

Class Outcomes

1. Assess the impact of AI on materials research and discovery
2. Selection of appropriate optimisation strategy for a given problem

Activity:

Closed-loop optimisation