Technische Universität Berlin

BAM Bundesanstalt für Materialforschung und -prüfung

Sicherheit in Technik und Chemie

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DATA DRIVEN MATERIALS DESIGN

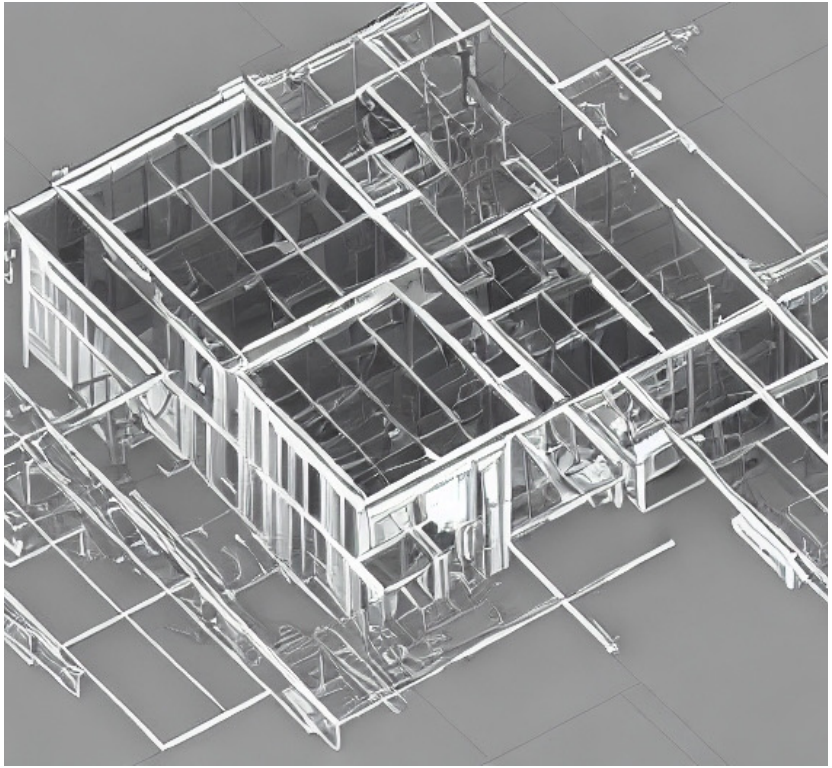
Dr. Christoph Völker

christoph.voelker@bam.de

www.bam.de

Abstract

The integration of computer modelling into the field of civil engineering has resulted in a transformative shift, allowing designers to simulate and evaluate their designs with unprecedented precision and cost-efficiency. While this advancement has significantly expanded design capabilities, the materials used in construction have yet to be fully incorporated into this digital revolution. This lecture series aims to bridge this gap by introducing AI-based techniques for materials design, providing a powerful solution for optimizing the selection and performance of materials in the built environment.



Short overview about BAM
Federal Institute for Materials Research and Testing

BAM

Federal Ministry
for Economic Affairs
and Climate Action

Federal departmental research institution, assigned to the Federal Ministry of Economics and Climate Protection (BMWK)

Task: Safety in technology and chemistry

Focus Areas: Energy, Environment, Infrastructure, Materials, Analytical Science

Employees: ca. 1500

Junior Research Group: Materials Characterization and Informatics for Sustainability in Construction

Head of Working Group/
Junior Professor
Sabine Kruschwitz

Deputy
Christoph Völker

Non-destructive material characterization to accelerate the development of green/sustainable building materials through

- the development of new approaches for the evaluation of durability properties
- The development of efficient tools to characterize the early hydration behavior / rheology of resource-efficient cementitious mixtures.
- The development of multi-methodological classification of construction waste to support the circular economy.

Material informatics for

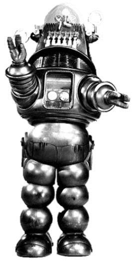
- Accelerating the development of environmentally friendly building materials through an AI-based approach
- AI software development for material science applications
- Creation, integration, enrichment and use of semantic material data structures

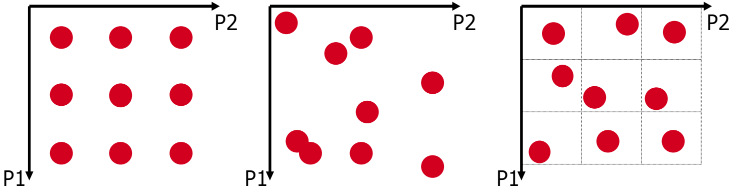
Scope

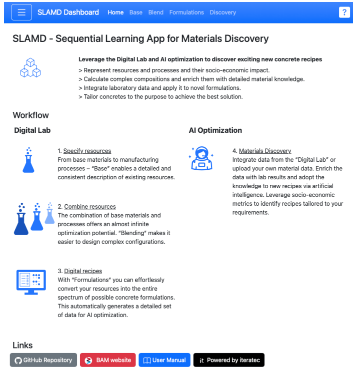
I. Introduction to data driven materials design
- Digital materials
- Model based prediction making
- Decision making

II. Advanced methods (next week)
- Creating digital materials
- Optimization strategies

III. Hands on (in two weeks)
- AI-driven materials design with SLAMD







Motivation

Challenges for the development of sustainable building materials

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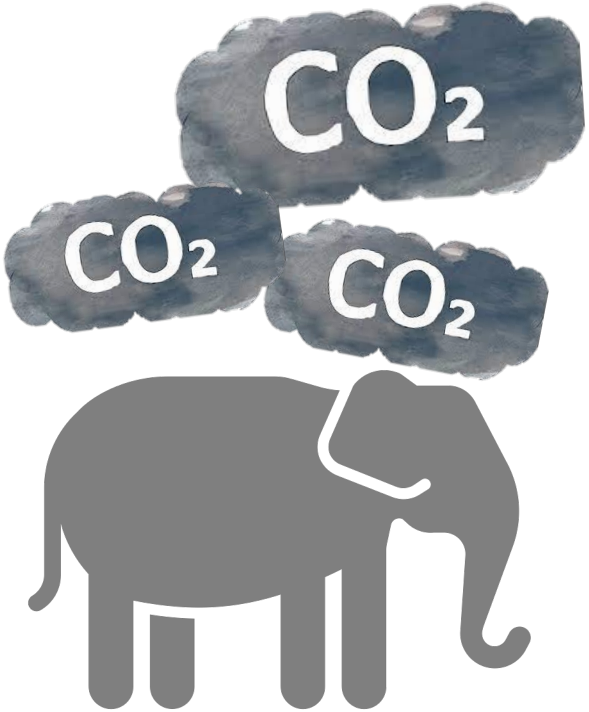
Ecological re-engineering of concrete necessary

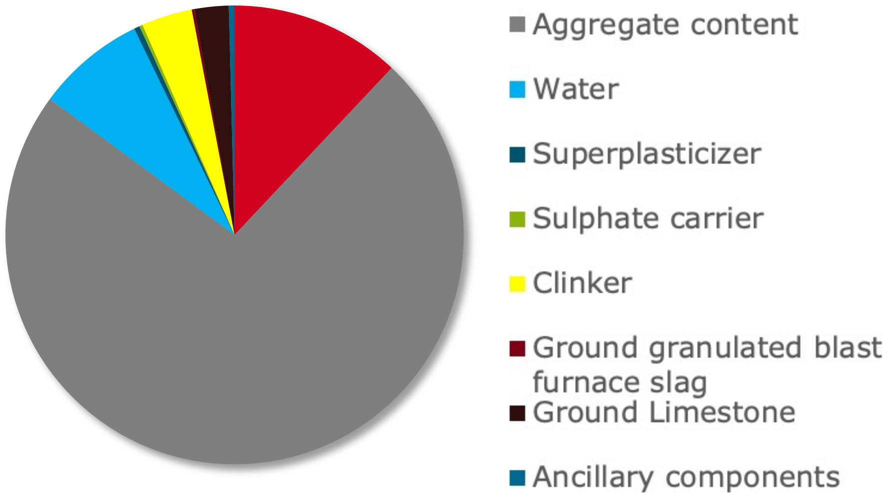


8% of man made

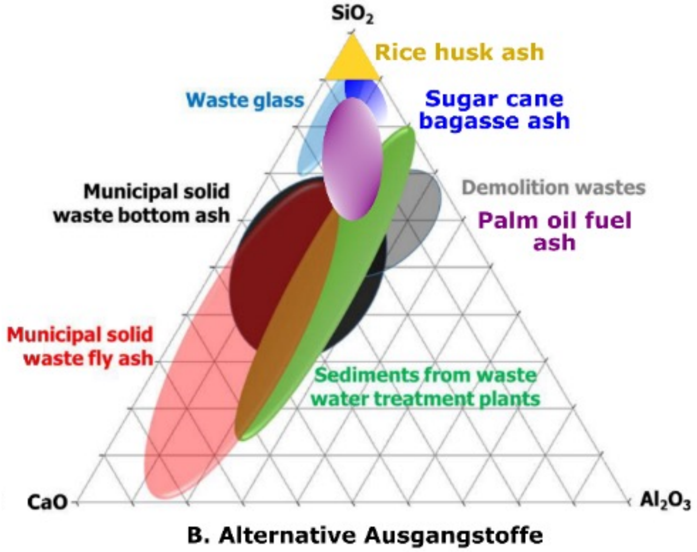
CO_2 come from cement

production *

Materials Complexity

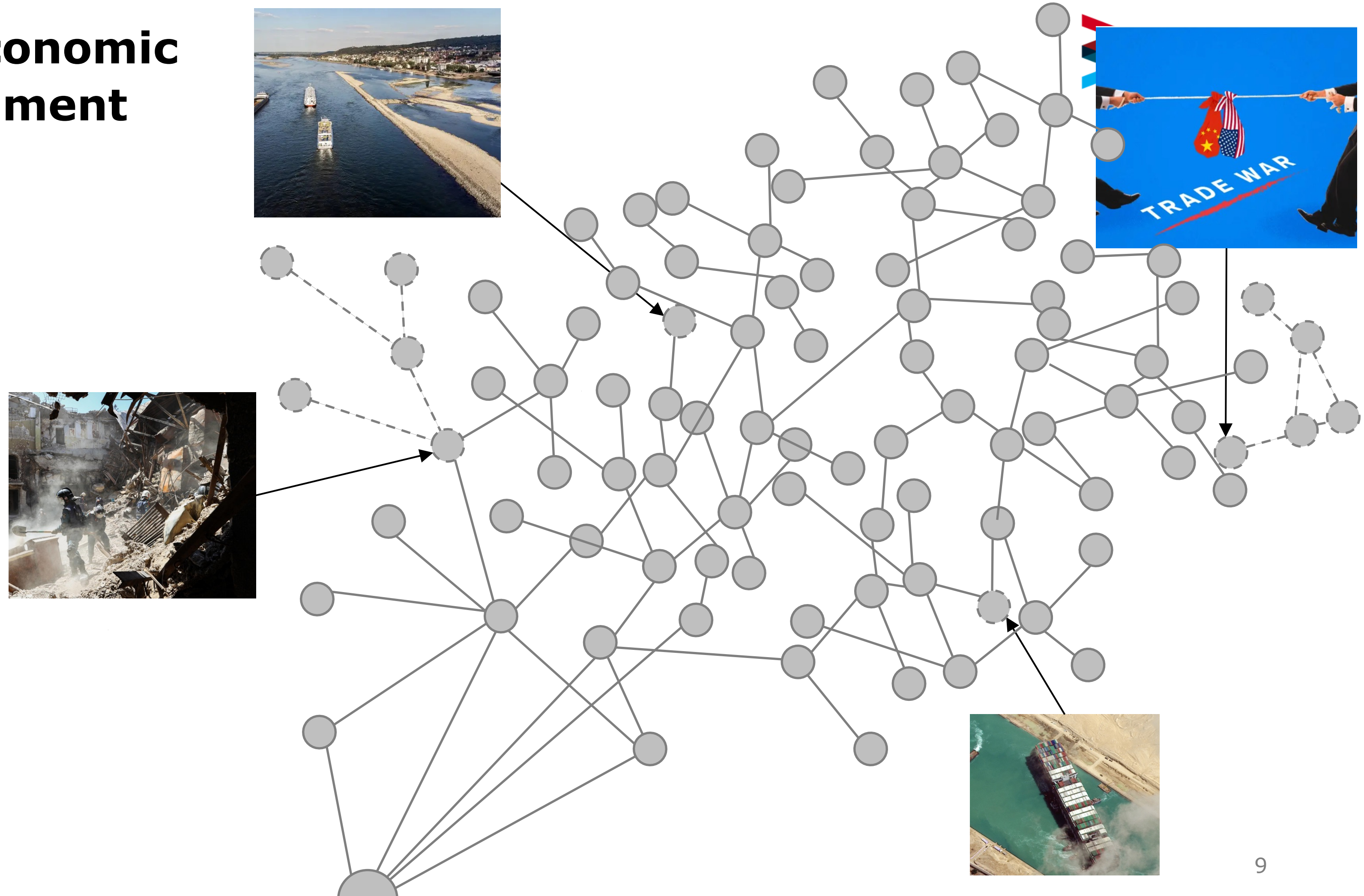


Composition complexity



Ressource inconsistency

Socioeconomic environment



Materials parameters

💪 Strength

🏃 Durability

🏗 Processability

…

Socioeconomic factors

🍀 Sustainability

💰 Costs

♻️ Resources & supply chains

…

Data driven materials design

Computer design

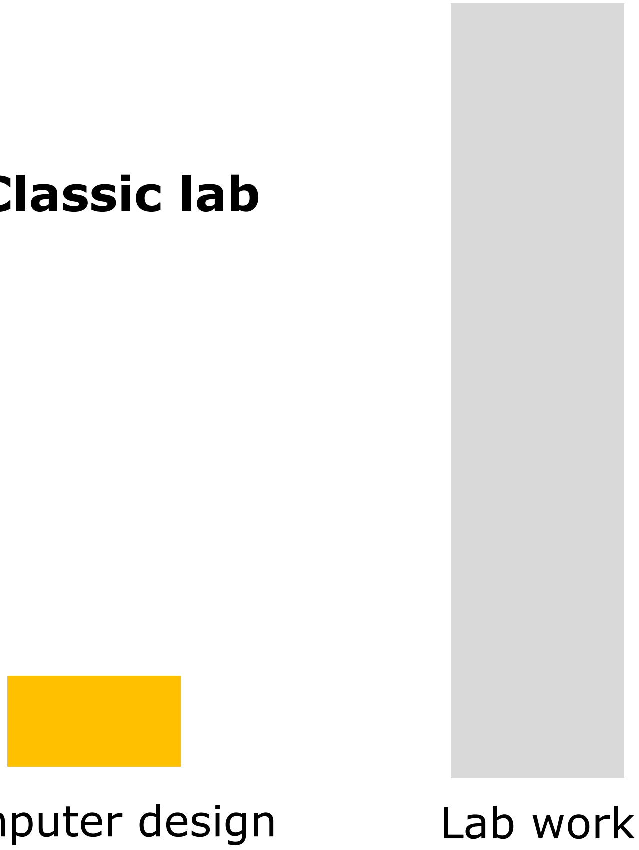
Predict

Validate

Lab work

Data driven materials design

Classic lab



expensive

time-consuming

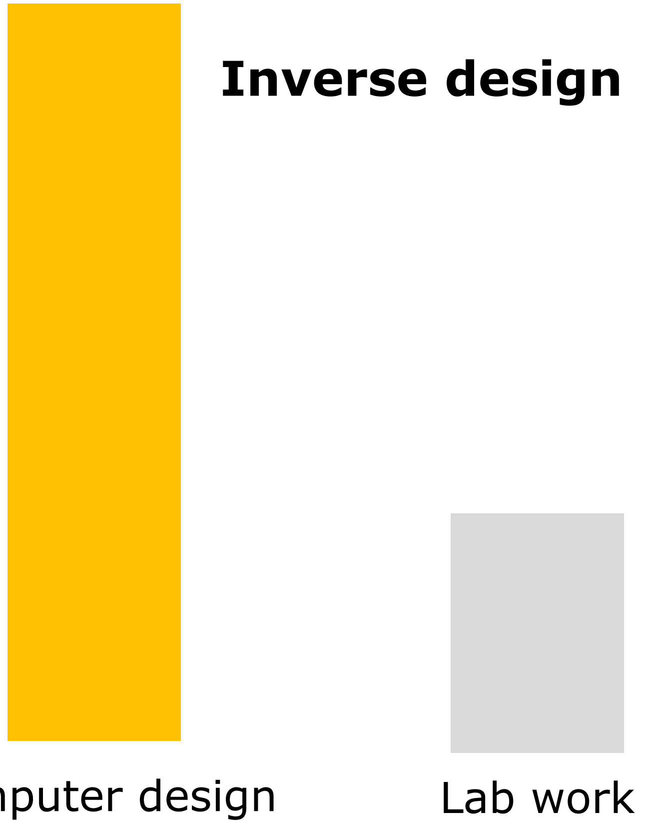
limited capacity

Data driven materials design

virtually free

lightning fast

virtually
unlimited
capacity



Inverse design

Autonomous materials design

virtually free

lightning fast

virtually unlimited capacity

Inverse design

+ proxy experiments
(for leads generation)

infinite testing

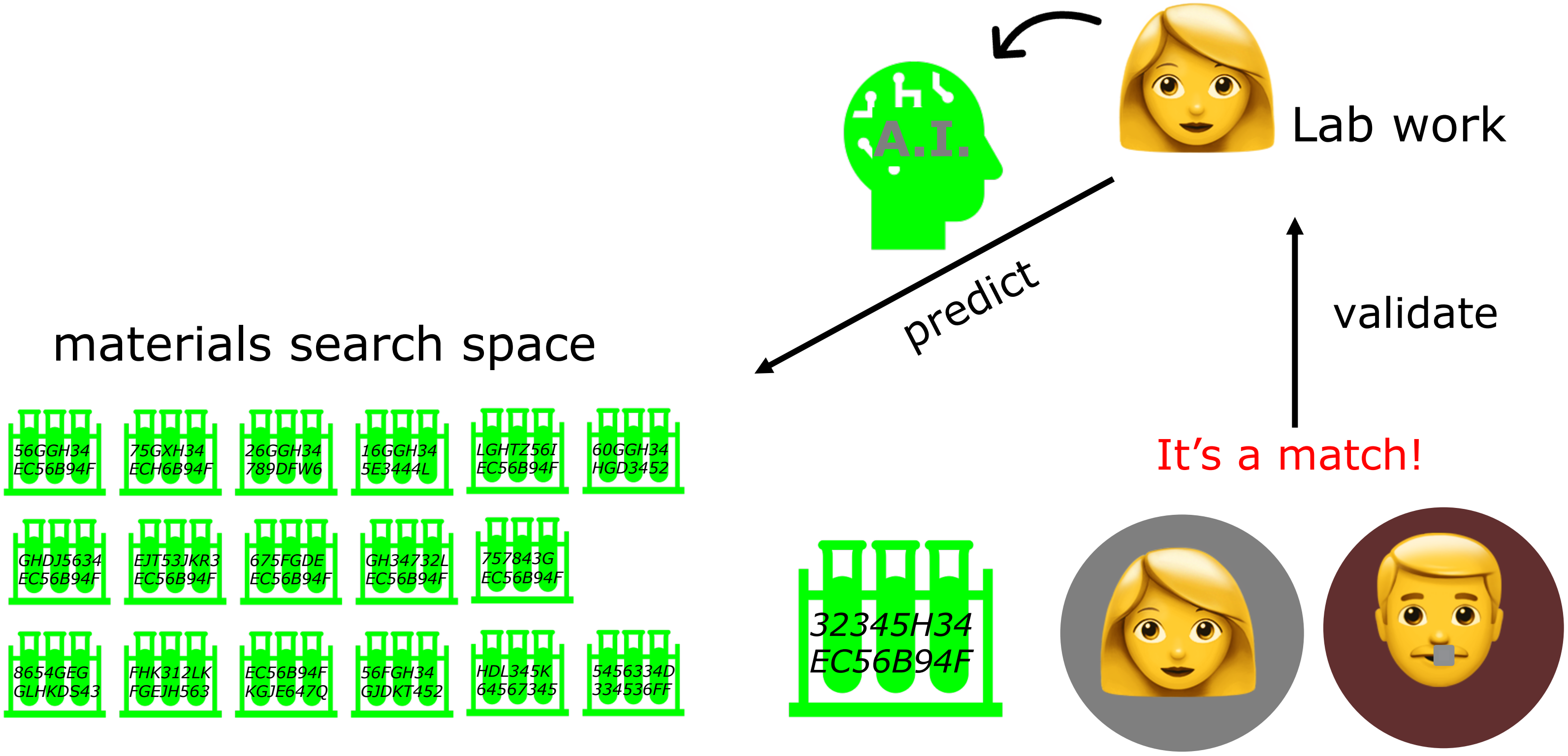
quick testing

simple automation

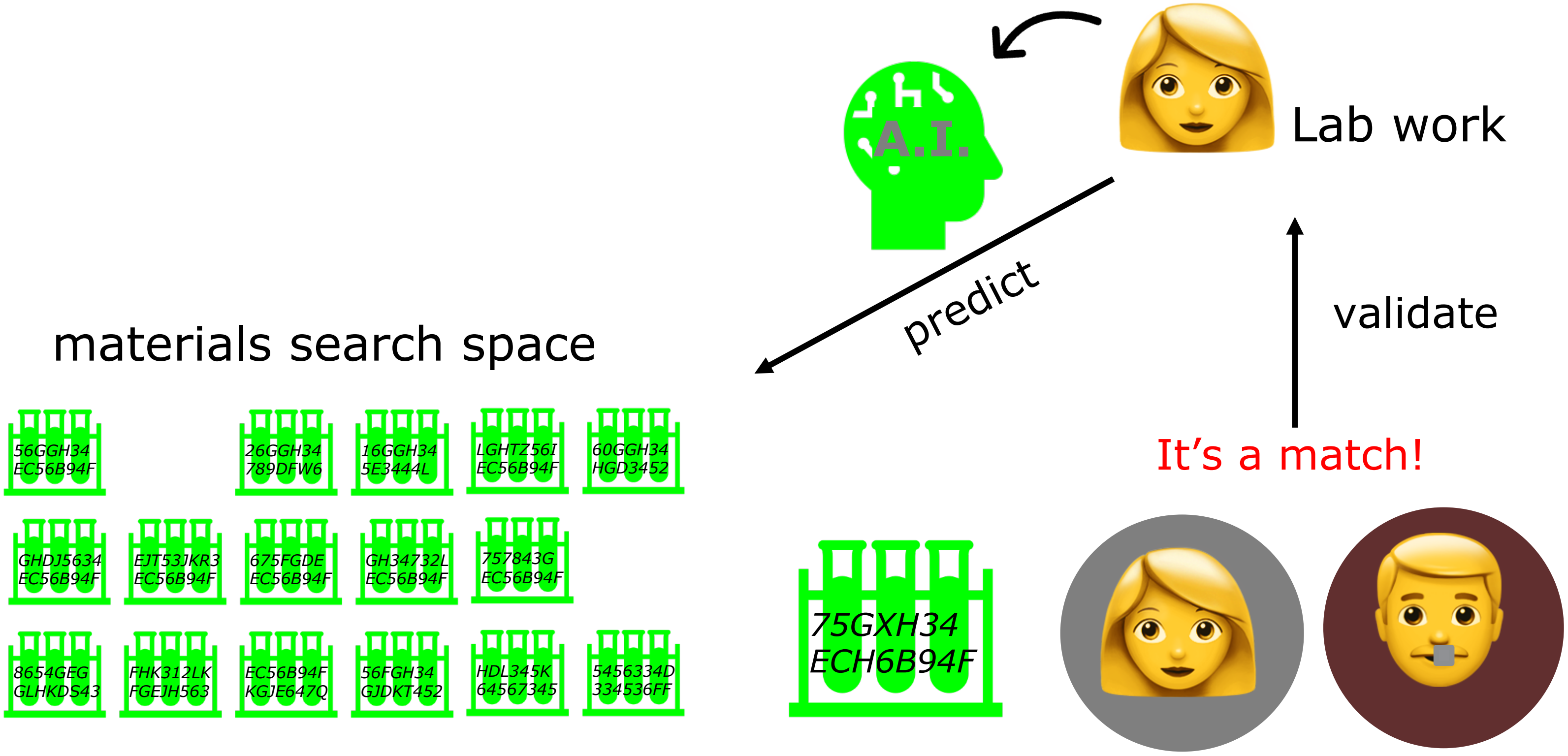
Computer design

Lab work

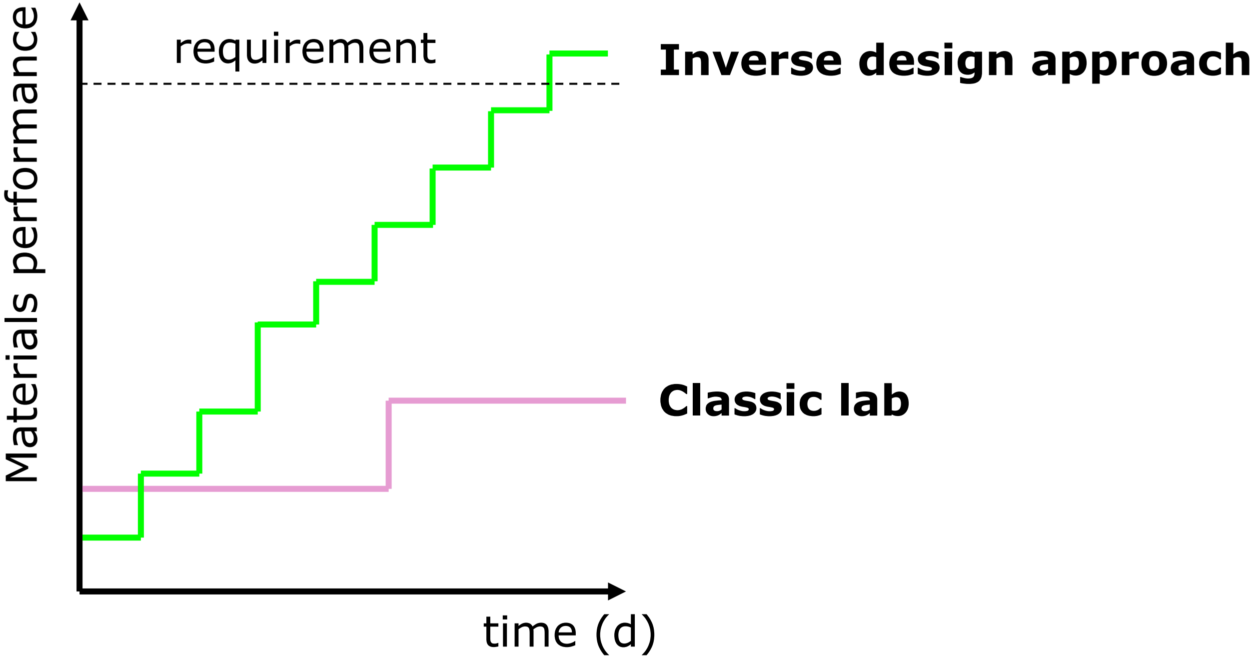
Inverse design



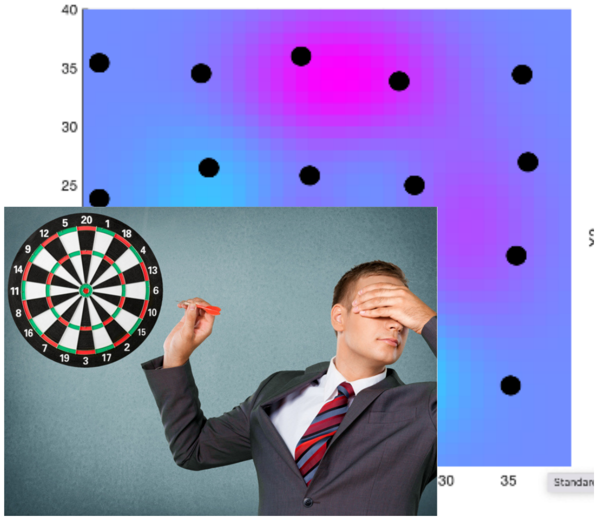
Inverse design



Autonomous materials development



Screening (traditional approach)

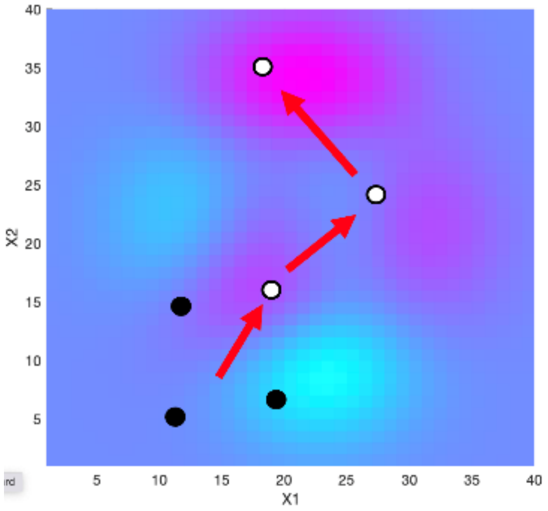


Screening a number of materials (black dots) according to the available resources to find the desired materials (pink areas).

But:

Too expensive! Exploring the numerous possible designs is not feasible.

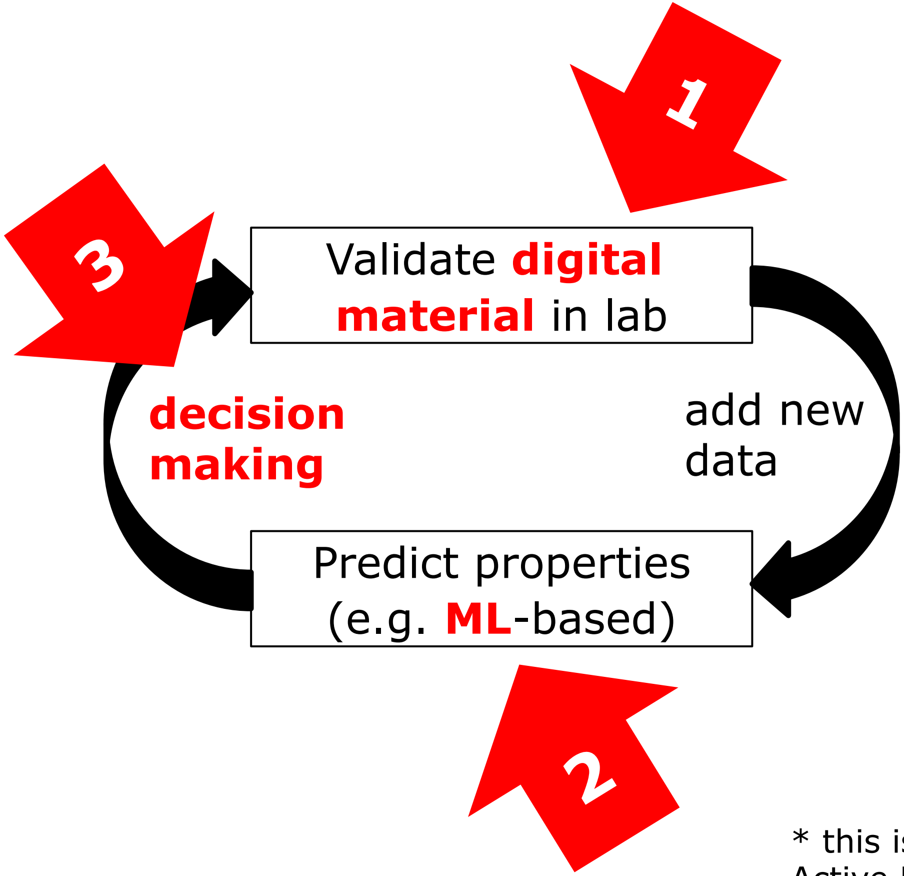
Inverse design



Iterative use of a predictive model (red arrow) to guide the experiments towards desired materials (pink areas).

Reducing the number of required experiments (black dots)

Inverse design workflow



Iterative feedback loop between the laboratory validation (e.g. with non destructive testing) of **digital materials** and the **ML** based prediction of properties via a **decision making** strategy.

* this is referred to as: Sequential Learning, Adaptive Sampling, Active Learning, Bayesian Optimization…

1. Digital materials

… describing materials with numbers

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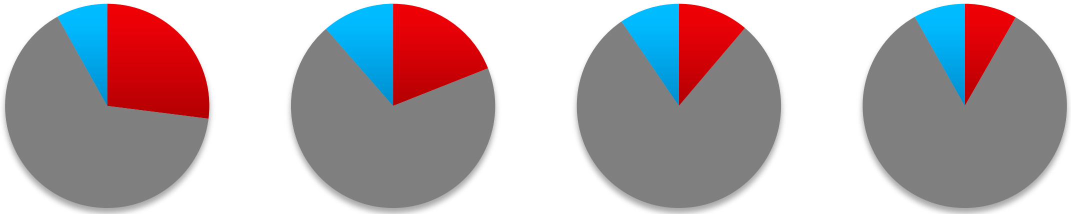
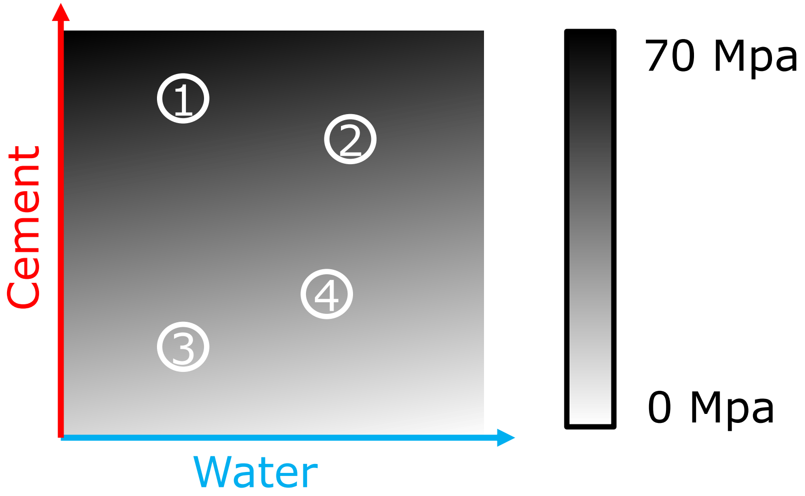
Digital materials



Recipe	1	2	3	4
Cement (kg/m^3)	540	380	166	224
Water (kg/m^3)	162	228	163	190
28 day strength (Mpa)	62	???		25

Digital materials



Recipe	1	2	3	4
Cement (kg/m^3)	540	380	166	224
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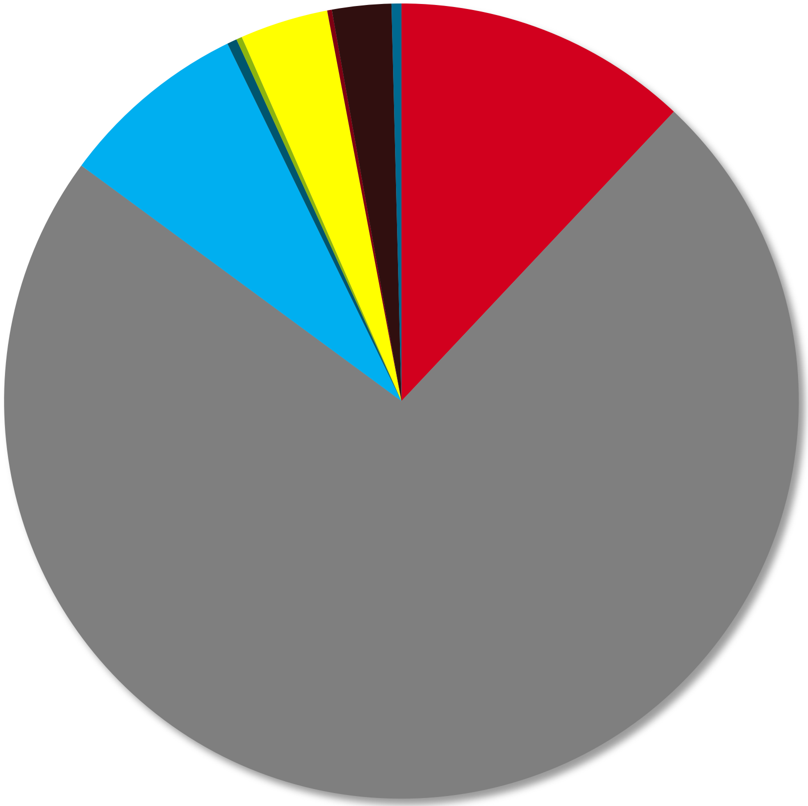
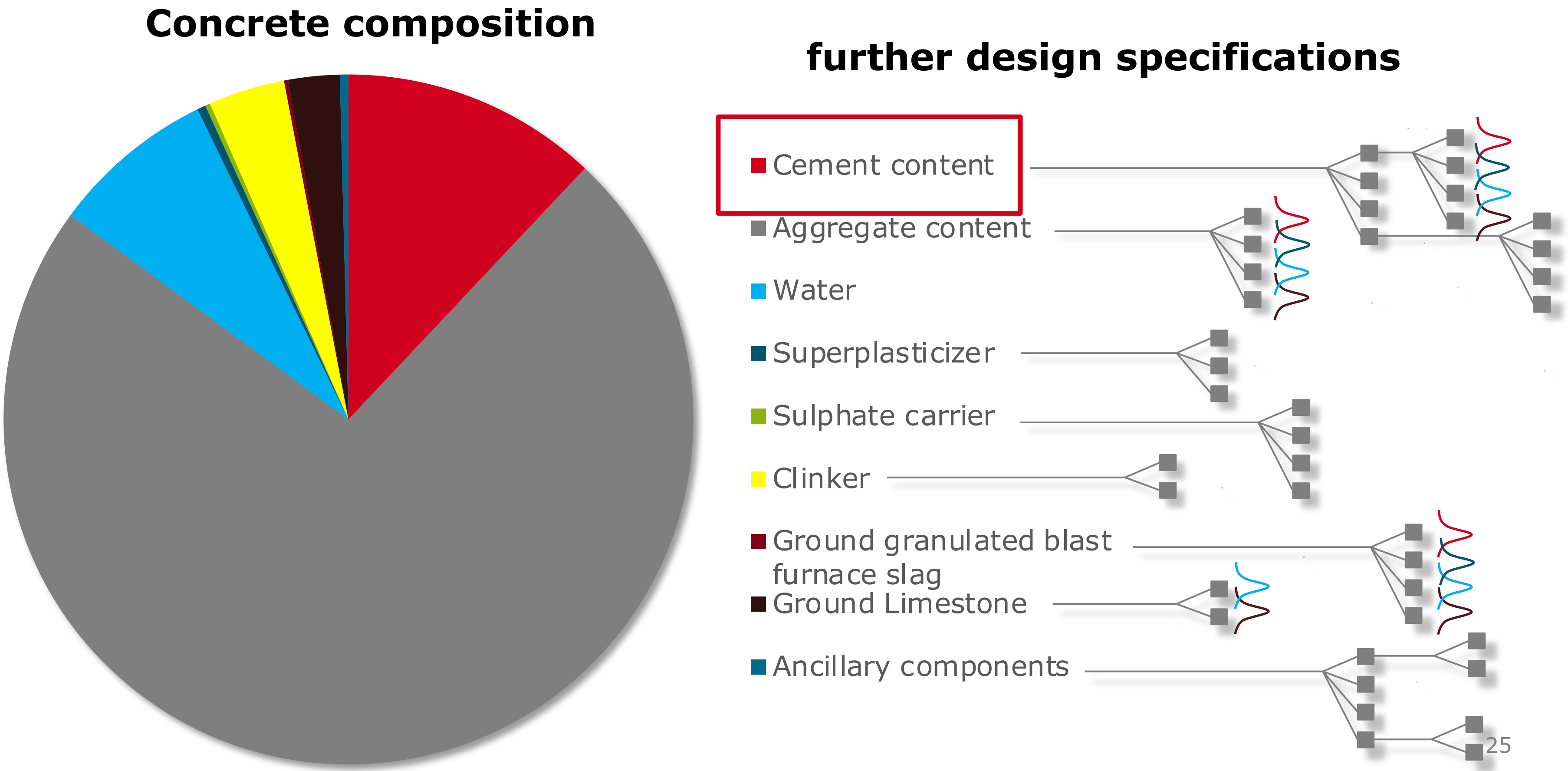
Digital materials

Concrete composition



Cement content	300 kg
Aggregate content	1823 kg
Water	192 kg
Superplasticizer	0.1 kg
Sulphate carrier	5,8 kg
Clinker	89,5 kg
Ground granulated blast furnace slag	4,7 kg
Ground Limestone	60 kg
Ancillary components	1 kg

Digital materials



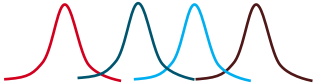
Digital materials

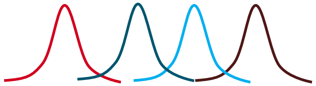
further design specifications may include:

- Cement content

Cement Type (CEM I, CEM II, CEM III, CEM IV,…)

Cement Plant (Berlin, Bochum, Munich, Prague,…)

Blaine Fineness 

Cement Composition 

Summary digital materials

- Digital materials describe relevant information of the **processing**, **structure** and **properties** of feasible materials.
- They are the basis for the AI prediction making

- Digital Materials typically consist of:
  - Parameters (controllable), e.g. concrete composition (weight fractures), curing time, heat treatment time, heat treatment temperature, mixing time, etc.
  - Properties (characteristic of a material or process), e.g. molecular composition, finness, density, strength, costs, CO_2 footprint, etc.
  - Conditions (uncontrollable), e.g. humidity, curing temperature, etc.

Example 1 from practice

OPC-based concrete with 32 entries

Idx	Zement	Werk	Beton	Zement Gehalt [kg/m³]	Gehalt Gesteinsk örnung [kg/m³]	Masse [kg/m³]	w/z	Fließmitt el [kg/m³]	Blaine	Sulfat-träger	Klinker	Neben-bestand-teile	HSM
1	CEM I 42,5 R	W1	C20/25	300	1823	2315	0,64	-	3000	6	89	5	0,0

KSM	BOS	CaO	SiO_2	Na2O-eq.	Fe_2O_3	MgO	Al_2O_3	SO_3	Sulfat-träger	Anhydrate	Halbhydrat	Gips	C_3S	C_2S	C_3A	C_4AF	Zement Preis [€/t]	GWP [CO2/t]
0,0	0,0	63	20	1	2	1	5	4	5	2	1	1	66	9	11	3	80	600

12 Parameters (controllable)

20 Properties (characteristic of a material or process)

0 Conditions (uncontrollable)

Example 2 from practice

BAM

Alkali-activated (green) concrete with 33 entries

Idx_Sample	SiO2	Al2O3	Fe2O3	CaO	MgO	Na2O	K2O	SO3	TiO2	LOI	FA (kg/m3)	GGBFS (kg/m3)	Coarse aggregate (kg/m3)
1399	52.295	24.571	3.215	12.58	3.242	154	0	515	0	3.391	252	108	1090.8

Fine aggregate (kg/m3)	Na2SiO3	NaOH	Na2O (l)	Sio2 (l)	H2O	Na2O (Dry)	Sio2 (Dry)	Water
774	115.7142857	46.28571429	115	0.3	0.59	13.31	34.71	67.69285714

Concentration (M) NaOH	Water	NaOH (Dry)	Additional water	Superplasticizer	water -eff	Initial curing time (day)
8	31.47428571	14.81142857	0	14.4	107.8071429	0

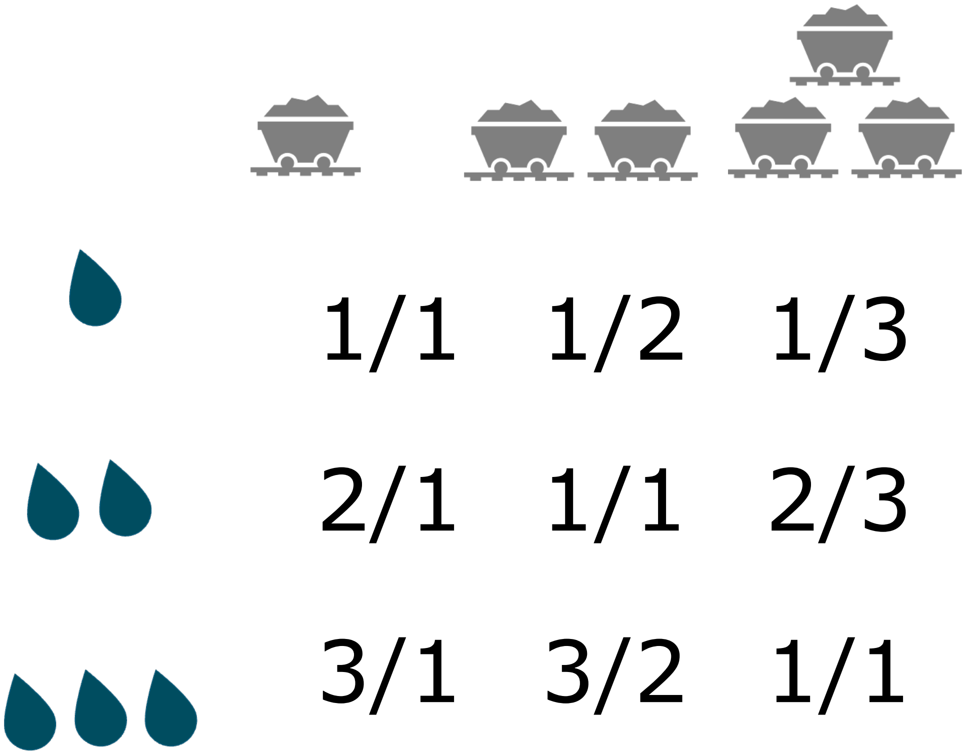
Initial curing temp (C)	Initial curing rest time (day)	Final curing temp (C)	Mixture CO2 (Na2SiO3 as solution)
25	1	30	112.66806856355

16 Parameters (controllable)

16 Properties (characteristic of a material or process)

1 Condition (uncontrollable)

Numeric example

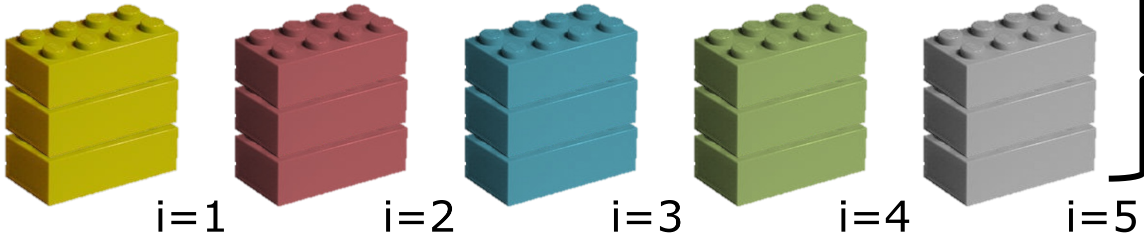


Digital Materials

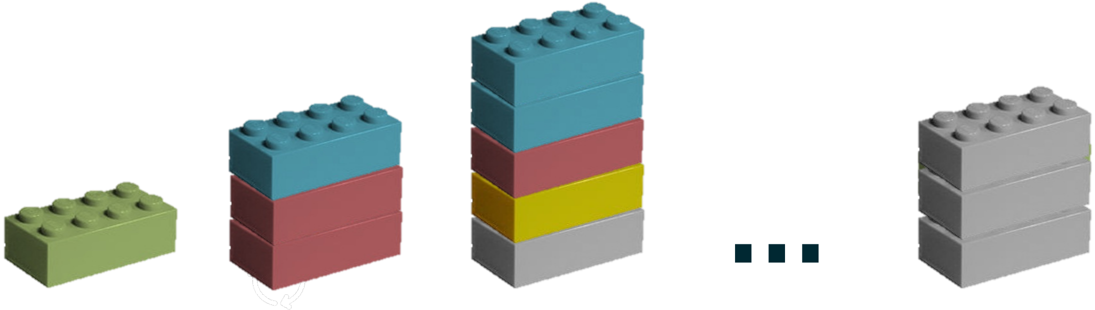
Liquid (wt.%)	Powder (wt.%)	CaO (wt.%)
50	50	12
33	66	12
25	75	12
20	80	12
66	33	12
75	25	12
80	20	12

How many Lego materials can we create…

… when these blocks symbolize possible materials parameter



$$\left.\right\} Range\ \mathfrak{R} = 4$$



$$N = \prod_{i=1}^{k} \mathfrak{R}_i - 1$$

Digital materials are a **virtually free resource** and can represent all kinds of designs. Finding the right design, however, is like the proverbial search for a **needle in the haystack**:

There are many possible materials (hay)

Only a few are well suited (needles)

2. Machine Learning (ML) for property prediction

… to make (cheap) virtual experiments

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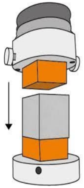
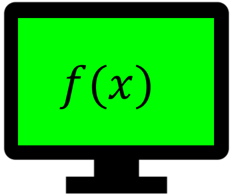
Intuition ML

Changes in the inputs (composition & processing) affect the outputs (properties).

ML can learn the relationships between inputs and outputs to predict properties of new material (with some margin of error).

Inputs	***System***	***Outputs***
Composition & processing	*Synthesis*	*Measured properties*
		
Digital materials	*ML-Model*	*Predicted properties*
$x =$ 		$y = f_{c,28d}$

Intuition parametric-Model $f(x)$

1. Training (on known materials):

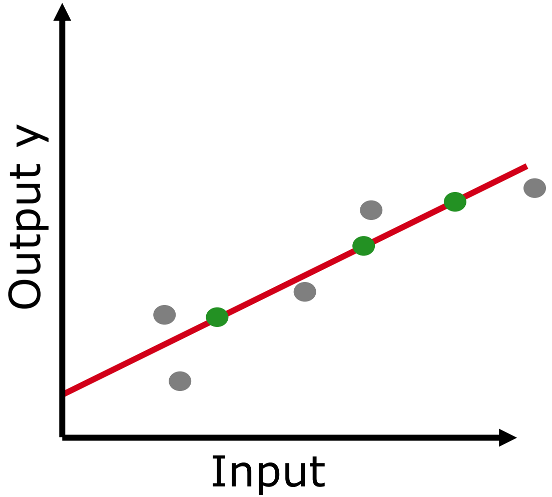
Fitting a linear function between inputs x and an output y by adjusting the model parameters b_0 and b_1 for the intercept and slope.

$$f\,(x) = b_0 + b_1 x$$

2. Prediction (for new materials):

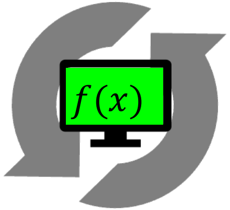
Apply model according to the following equation:

$$y = b_0 + b_1 x_1$$



1. ML training

Training Data
(digital materials)



Target
(from the lab)

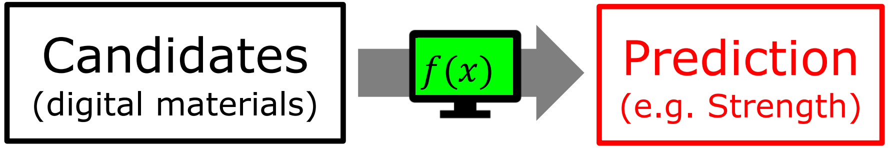
#	Para. 1	Para. 2	Para. 3	...	Para. N
1	12	154	I		x
2	2	12	O		y
⋮					
n	48	5	I		x

#	Target
1	10.1
2	0.8
⋮	
n	5.3

Fit ML *model parameters* between training data and targets.

Model performance = error between model output and (known) targets.

2. ML prediction



#	Para. 1	Para. 2	Para. 3	...	Para. N
1	155	0	O		X
2	1	0	O		u
...					
n	10	55	I		f

#	E(P=1,X)	Uncertainty std(E)
1	3.9	0.1
2	10.8	0.13
...		
n	12.2	2.0

Prediction of the expected properties (E) of candidates with unknown properties. The uncertainty of each prediction can be derived by statistical methods*.

*introduction here: https://www.inovex.de/de/blog/uncertainty-quantification-deep-learning/

3. Decision making strategies

… making the best out of available information

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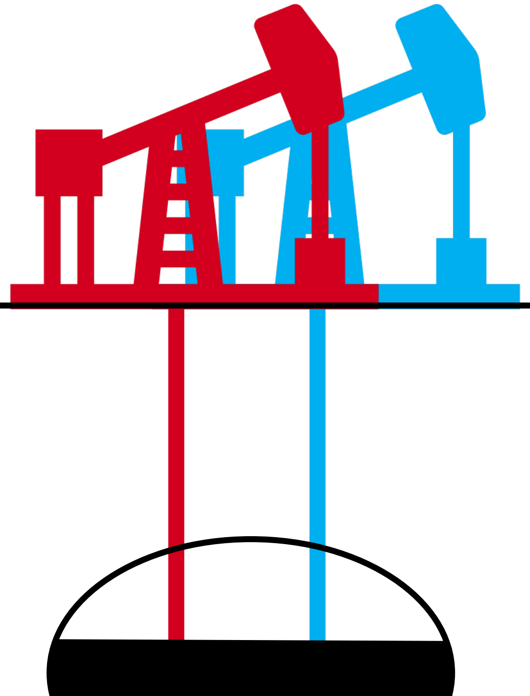
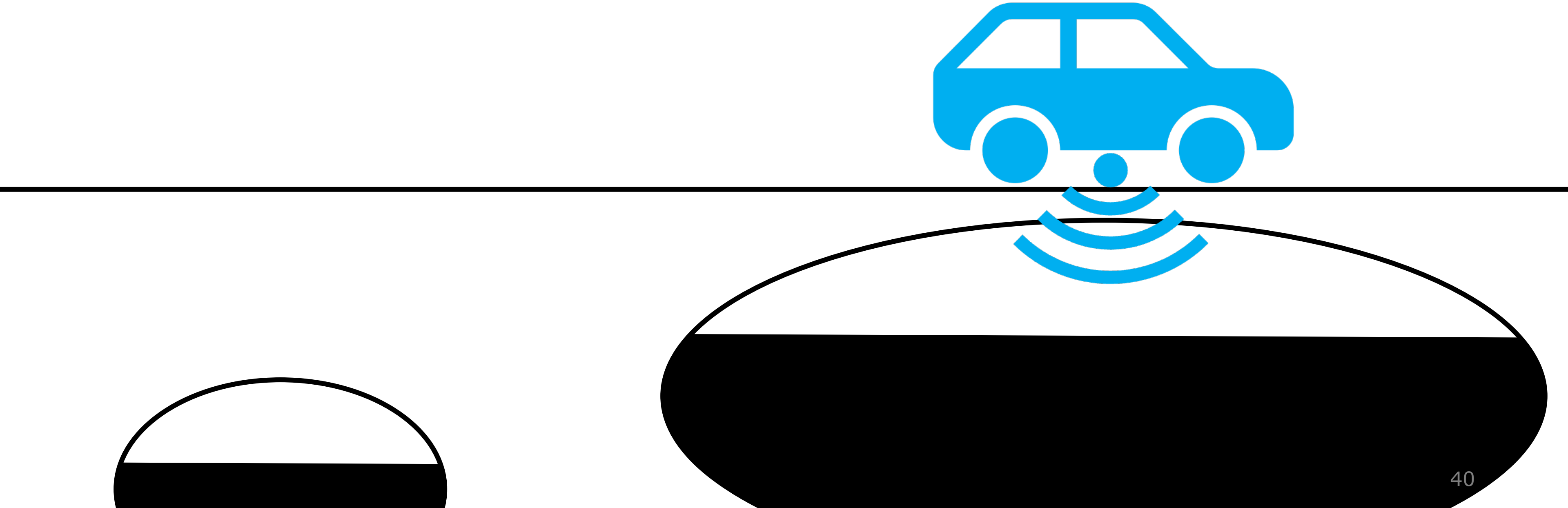
Intuition decision making

Exploit: Look for opportunities in proximity to what works well

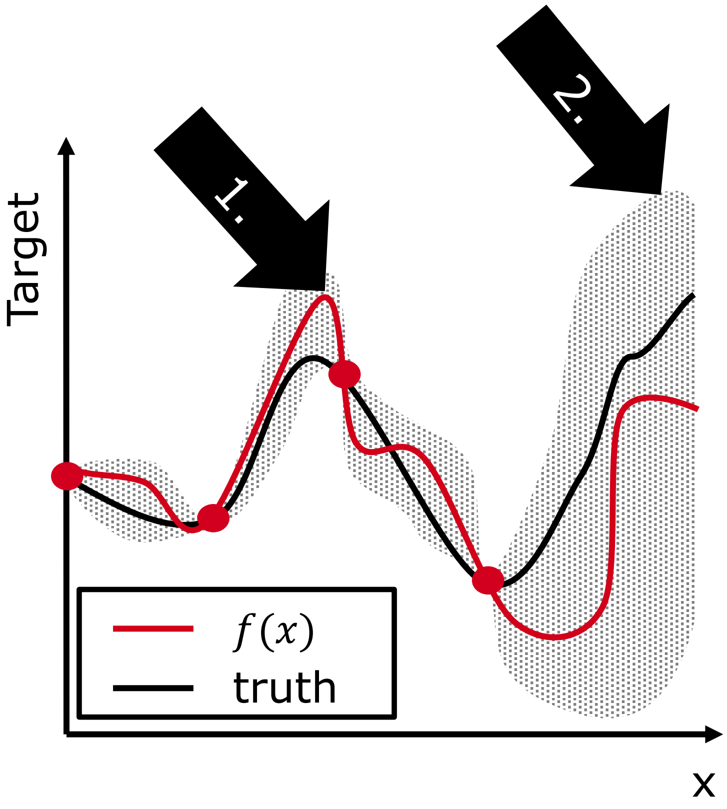


Intuition decision making

Explore: Seek opportunities in regions of high uncertainty



Intuition decision making



Actually, the outcome of an experiment is the deviation from what we expected

If the outcome of an experiment is already known, there is no reason to conduct it and an experiment can be more useful if the uncertainty of its outcome is large

1. Maximum expected performance

2. Maximum likelihood of performance

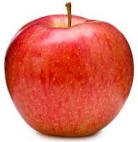
Decision making (target)

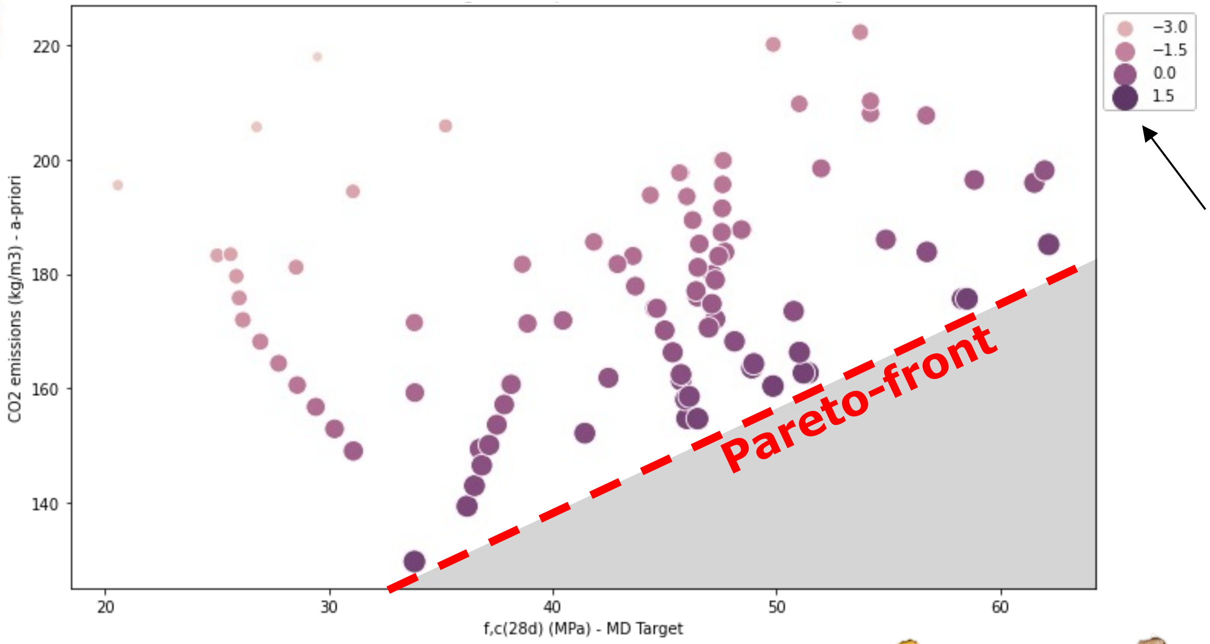
To find materials that are:

Target	**Property**
high strength	$Max(f,c(28\ d))$
good looking	$Min(Surface\ noise)$
workable	$Max(Slump)$
durable	$Min(CO_2 penetration\ KN)$
cheap	$Min(€)$
available	$Min(tdeliver_y)$
climate friendly	$Min(CO_2\ emission)$

Decision making (utility function)

Strength vs. carbon emissions with coloured utility





Utility is an abstract, measure that is usually estimated by a function

e.g. as the normalized (weighted) sum of target properties

Decision making (utility function)

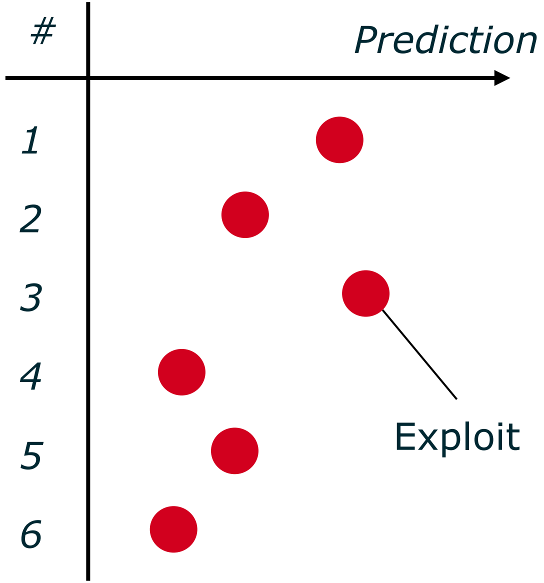
The maximum expected improvement (**MEI**) can be expressed by the utility function:

$$Utility_{MEI} = \sum_{i=1}^{N} w_i \bar{E}_i$$

Number of targets

To control the weight (a.k.a importance) of a target

Normalized expected/predicted performance



Decision making (utility function)

The maximum likelihood of improvement (**MLI**) can be expressed by the utility function:

$$Utility_{MLI} = \sum_{i=1}^{N} w_i(\bar{E}_i + u_i * \bar{\sigma}_i)$$

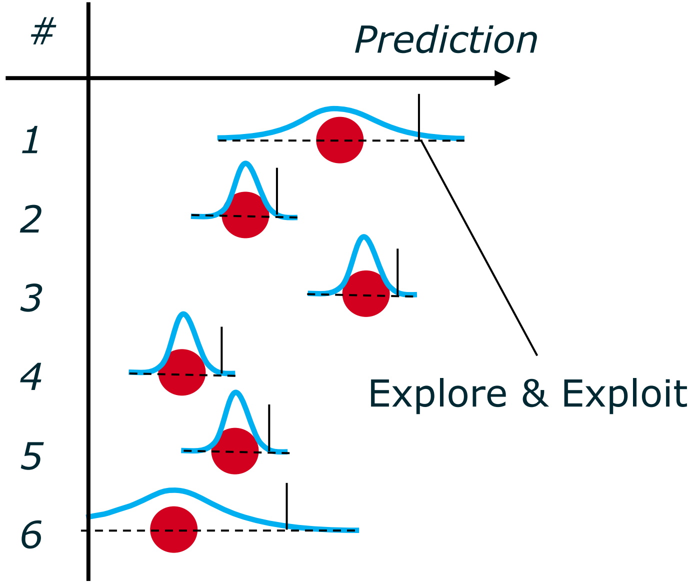
Number of targets

To control the weight (a.k.a importance) of a target

Normalized expected/predicted performance

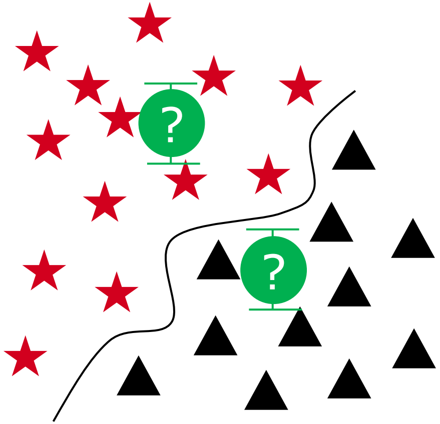
To control the degree of exploration

Predicted uncertainty, i.e. standard deviation



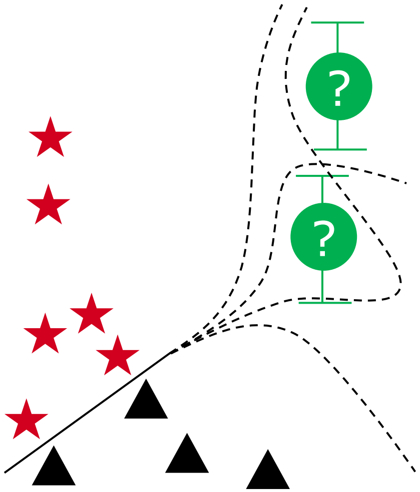
Intuition Decision making

Exploit (MEI)



Known materials

Explore (MLI)

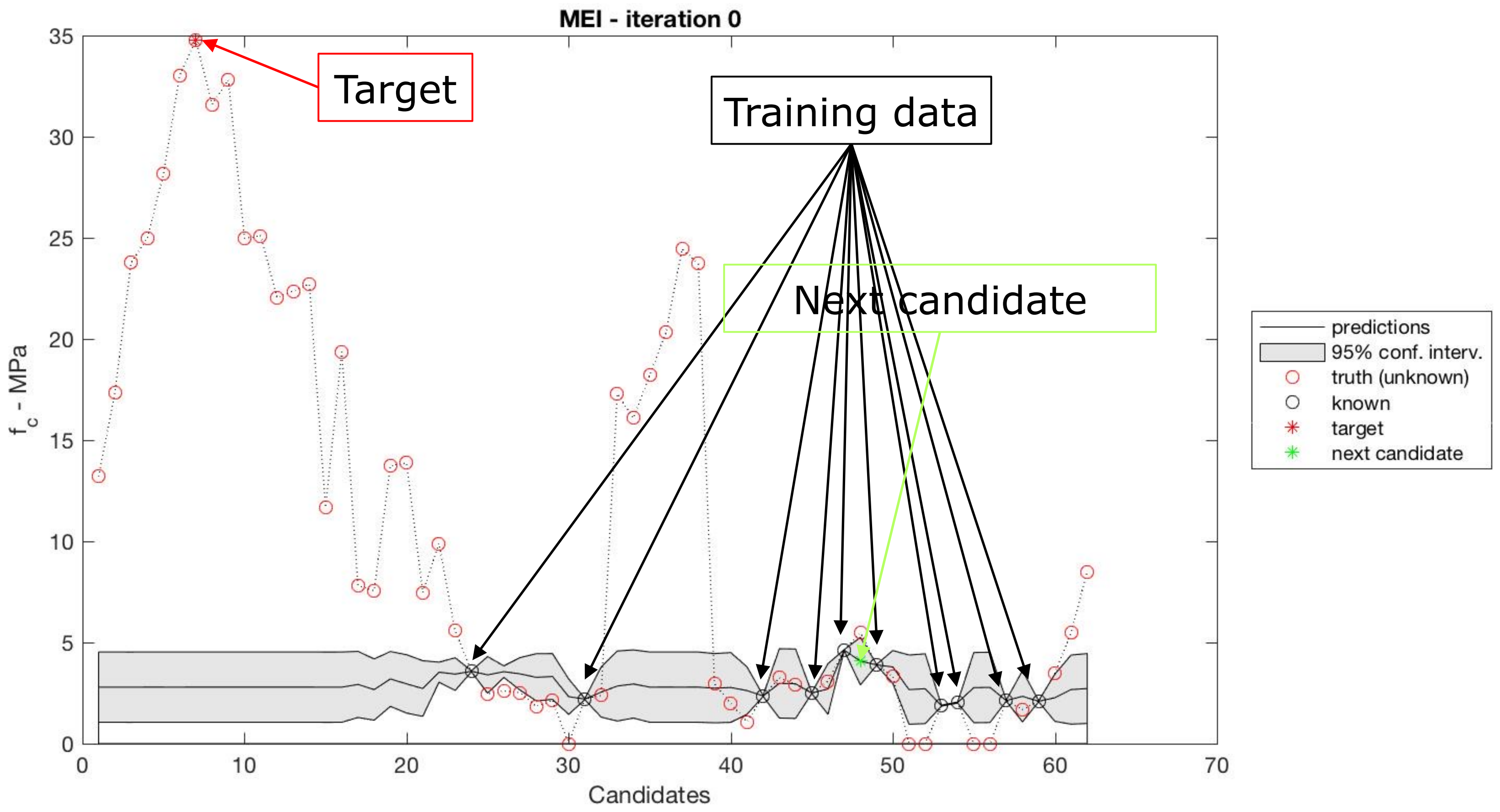


New materials

Summary

- **MEI** (pure exploitation)
  - when sufficient training data are available -> good model
  - when training data similar to candidates & models are certain
  - when deadlines are pressing
- **MLI** (explore and exploit)
  - to discover "moon-shot" materials (e.g. if predictions are not satisfying)
  - the weight of the uncertainty u_i can controls the extent to which the model explores
  - at the beginning of experimentation and for long-term studies (exploration)

Examples

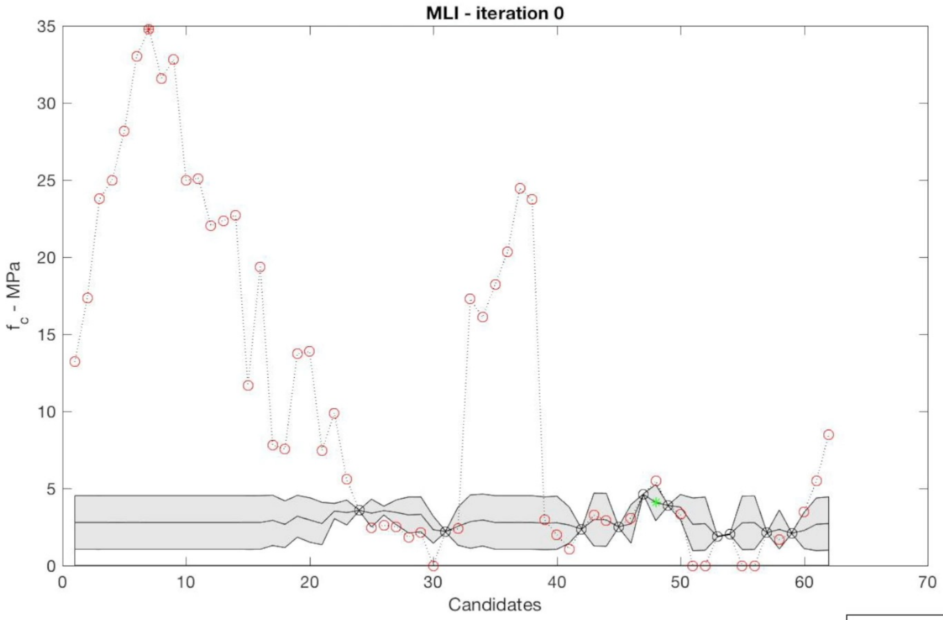


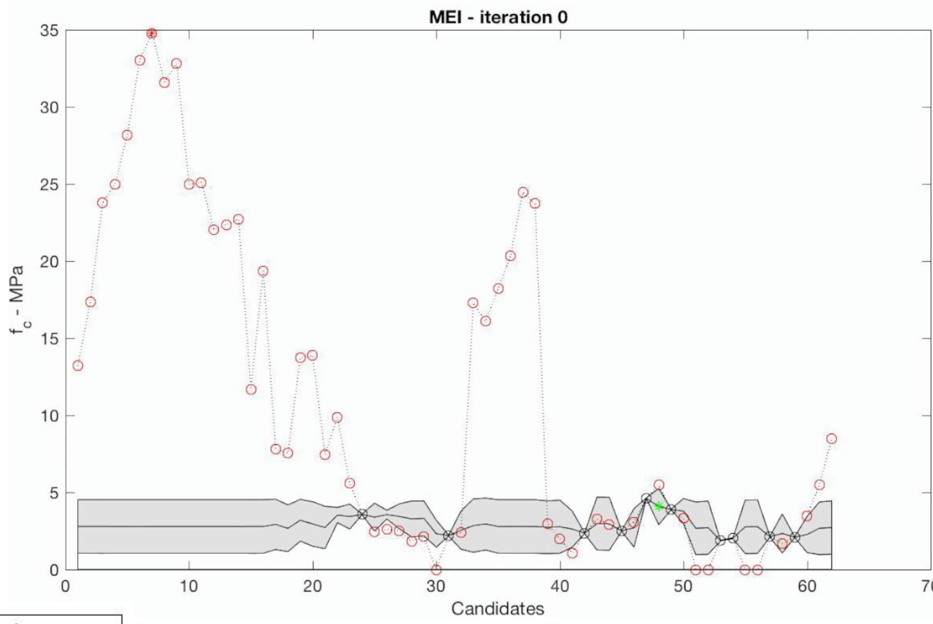
MEI - iteration 0
Target
Training data
Next candidate
predictions
95% conf. interv.
truth (unknown)
known
target
next candidate
f_c - MPa
Candidates
0
5
10
15
20
25
30
35
0
10
20
30
40
50
60
70

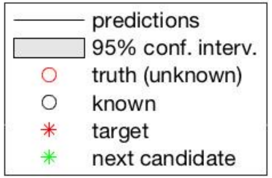
Examples

MLI („explore & exploit")

MEI („exploit")







4. Case studies: building materials and outlook

www.bam.de

1. Case Study PhD Thesis TU-B*

131 Alkali-Activated Binders from 3 Ph-D Thesis

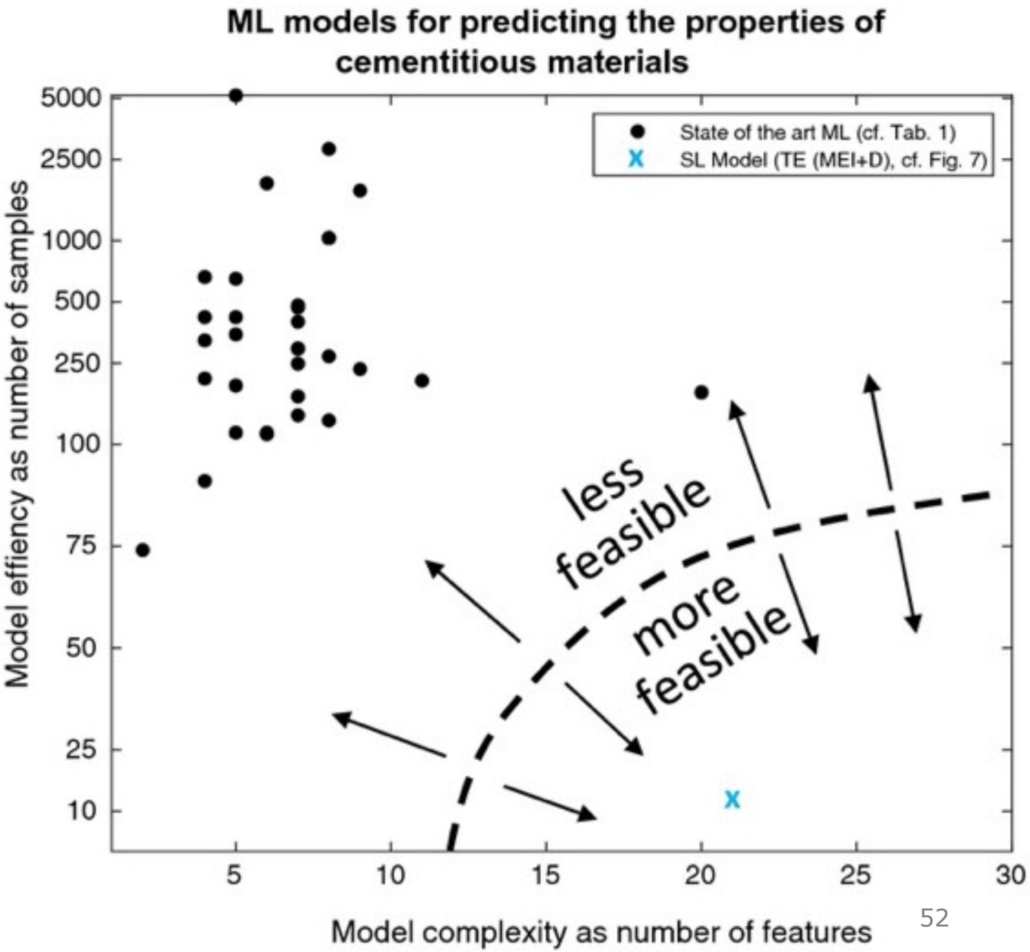
*Source: Völker et al. (2021) DOI: 10.1007/s10853-021-06324-z

Temperature (°C)	LOI	SiO_2	Al_2O_3	Fe_2O_3	MnO	MgO	CaO	Na_2O	K_2O	TiO_2	P_2O_5	SO_3	Cl	Blaine fineness (cm2/g)	d90 (µm)	d50 (µm)	Solution/ Powder	SiO_2 (mol-%)	Na_2O (mol-%)	K_2O (mol-%)	H_2O (mol-%)	Compressive strength (MPa)
22,00	6,50	50,20	17,48	5,10	0,22	1,51	8,76	4,03	4,79	0,67	0,20	0,47	0,00	6623,00	19,03	6,89	0,50	4,04	9,51	0,00	86,46	13,21
22,00	6,50	50,20	17,48	5,10	0,22	1,51	8,76	4,03	4,79	0,67	0,20	0,47	0,00	6623,00	19,03	6,89	0,50	3,91	7,96	0,00	88,14	17,32
22,00	6,50	50,20	17,48	5,10	0,22	1,51	8,76	4,03	4,79	0,67	0,20	0,47	0,00	6623,00	19,03	6,89	0,50	3,76	6,17	0,00	90,08	23,77
22,00	6,50	50,20	17,48	5,10	0,22	1,51	8,76	4,03	4,79	0,67	0,20	0,47	0,00	6623,00	19,03	6,89	0,50	5,98	8,45	0,00	85,57	24,98
22,00	6,50	50,20	17,48	5,10	0,22	1,51	8,76	4,03	4,79	0,67	0,20	0,47	0,00	6623,00	19,03	6,89	0,50	5,79	7,26	0,00	86,95	28,15
22,00	6,50	50,20	17,48	5,10	0,22	1,51	8,76	4,03	4,79	0,67	0,20	0,47	0,00	6623,00	19,03	6,89	0,50	5,85	6,19	0,00	87,96	33,03
22,00	6,50	50,20	17,48	5,10	0,22	1,51	8,76	4,03	4,79	0,67	0,20	0,47	0,00	6623,00	19,03	6,89	0,50	8,24	7,77	0,00	84,00	34,78
22,00	6,50	50,20	17,48	5,10	0,22	1,51	8,76	4,03	4,79	0,67	0,20	0,47	0,00	6623,00	19,03	6,89	0,50	8,06	6,95	0,00	84,99	31,59
22,00	6,50	50,20	17,48	5,10	0,22	1,51	8,76	4,03	4,79	0,67	0,20	0,47	0,00	6623,00	19,03	6,89	0,50	9,22	7,25	0,00	83,53	32,81
22,00	6,50	50,20	17,48	5,10	0,22	1,51	8,76	4,03	4,79	0,67	0,20	0,47	0,00	6623,00	19,03	6,89	0,50	8,36	6,39	0,00	85,25	24,98
22,00	6,50	50,20	17,48	5,10	0,22	1,51	8,76	4,03	4,79	0,67	0,20	0,47	0,00	6623,00	19,03	6,89	0,50	9,27	6,79	0,00	83,94	25,10
22,00	6,50	50,20	17,48	5,10	0,22	1,51	8,76	4,03	4,79	0,67	0,20	0,47	0,00	6623,00	19,03	6,89	0,50	9,07	6,05	0,00	84,88	22,05
22,00	6,50	50,20	17,48	5,10	0,22	1,51	8,76	4,03	4,79	0,67	0,20	0,47	0,00	6623,00	19,03	6,89	0,50	8,66	5,53	0,00	85,82	22,37
22,00	6,50	50,20	17,48	5,10	0,22	1,51	8,76	4,03	4,79	0,67	0,20	0,47	0,00	6623,00	19,03	6,89	0,50	9,14	5,33	0,00	85,53	22,73
22,00	6,50	50,20	17,48	5,10	0,22	1,51	8,76	4,03	4,79	0,67	0,20	0,47	0,00	6623,00	19,03	6,89	0,50	4,05	4,61	0,00	91,35	11,68
22,00	6,50	50,20	17,48	5,10	0,22	1,51	8,76	4,03	4,79	0,67	0,20	0,47	0,00	6623,00	19,03	6,89	0,50	6,20	4,99	0,00	88,81	19,37
22,00	11,24	52,35	12,25	4,15	0,09	0,91	13,85	1,67	2,44	0,61	0,22	0,27	0,00	6746,00	22,87	5,39	0,75	4,04	9,51	0,00	86,46	7,81

1. Case Study PhD Thesis TU-B

_11/131_

experiments to find good performance materials with high certainty



2. Literature Case Study*

- 9 data sets with 1367 alkali-activated concrete mixes
- 90 to 274 candidate materials
- 28 to 43 materials parameters
- Compressive strength and CO_2 footprint are optimized

Input data description				
Nr.	Shape, dimensions (mm)	Nr. of samples	Nr. of materials parameters	Testing age (days)
1	Cube, 100^3	105	39	1
2	Cube, 100^3	126	36	7
3	Cube, 100^3	188	43	7
4	Cube, 100^3	139	37	28
5	Cube, 100^3	250	43	28
6	Cube, 150^3	274	32	28
7	Cylinder, 100x200	105	28	7
8	Cylinder, 100x200	90	39	7
9	Cylinder, 100x200	90	38	28

*Source: Völker et al. (2022) DOI: 10.13140/RG.2.2.33502.92480/1

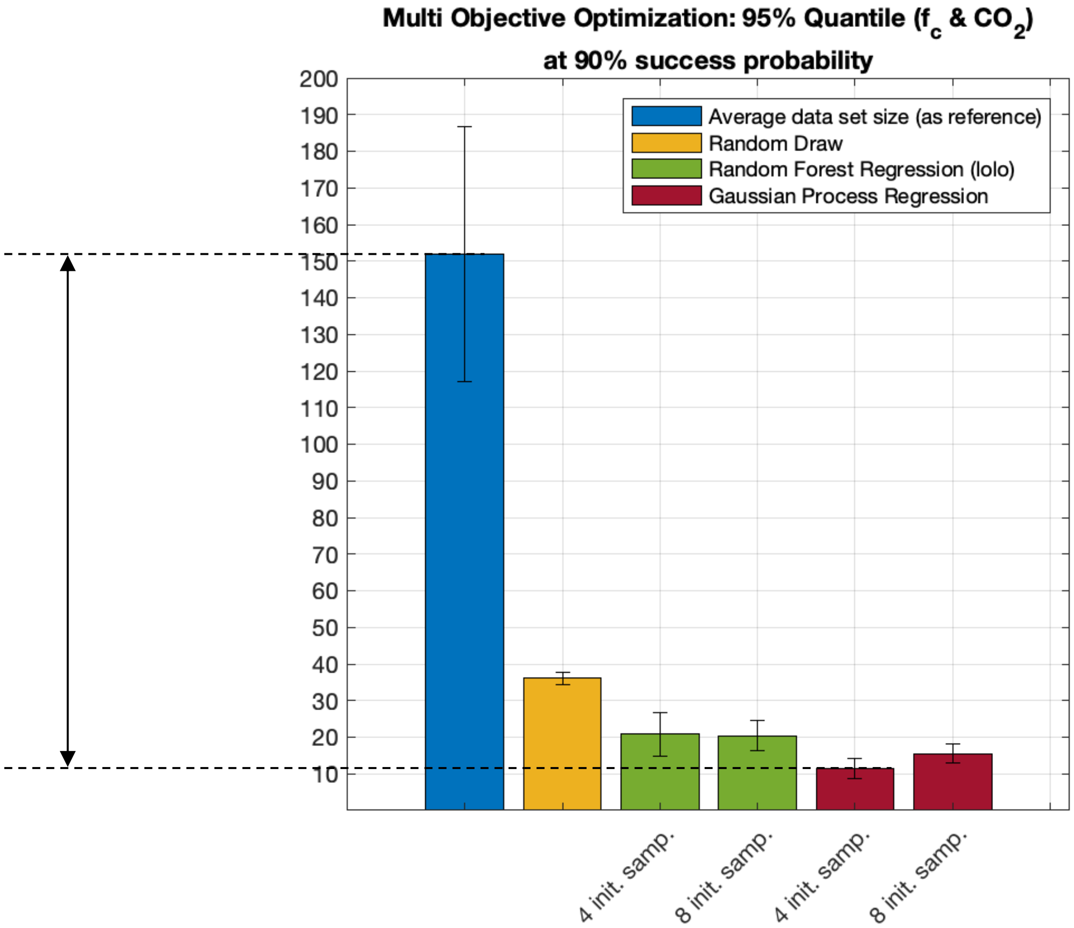
2. Literature Case Study

_>10 x_

more efficient

than classic

experiments



Autonomous materials development platforms

BAM

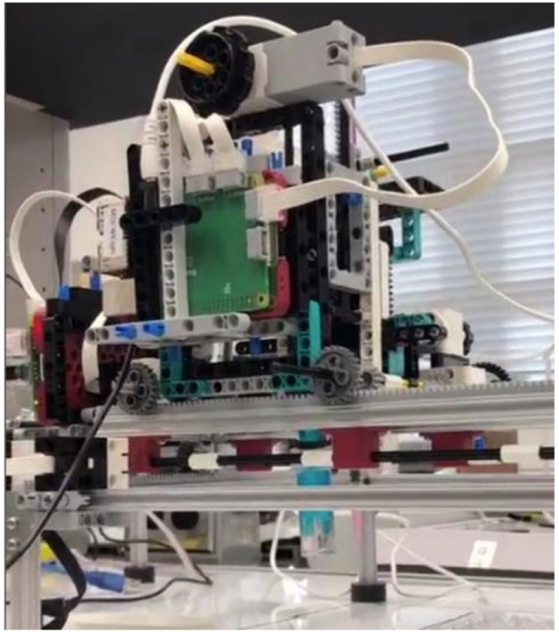
"Legolas" Low-Cost Robot Science Kit for Hypothesis Discovery and Validation

Built with Lego, 2 robotic axis, Raspberry Pi, 1 pump

Costs: < 300 $

Task:

Learn relationship between composition and PH-value



L. Saar et al. (2022)
https://doi.org/10.1557/s43577-022-00430-2
https://www.youtube.com/watch?v=TtPM7zXI5kQ

Autonomous materials development platforms

Atinary SDLabs Demo

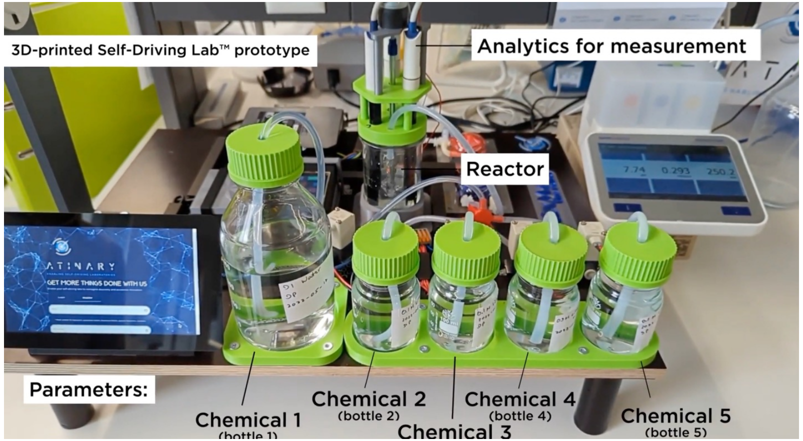
3D printed platform, 5 pumps

Costs: 500 $

Task:

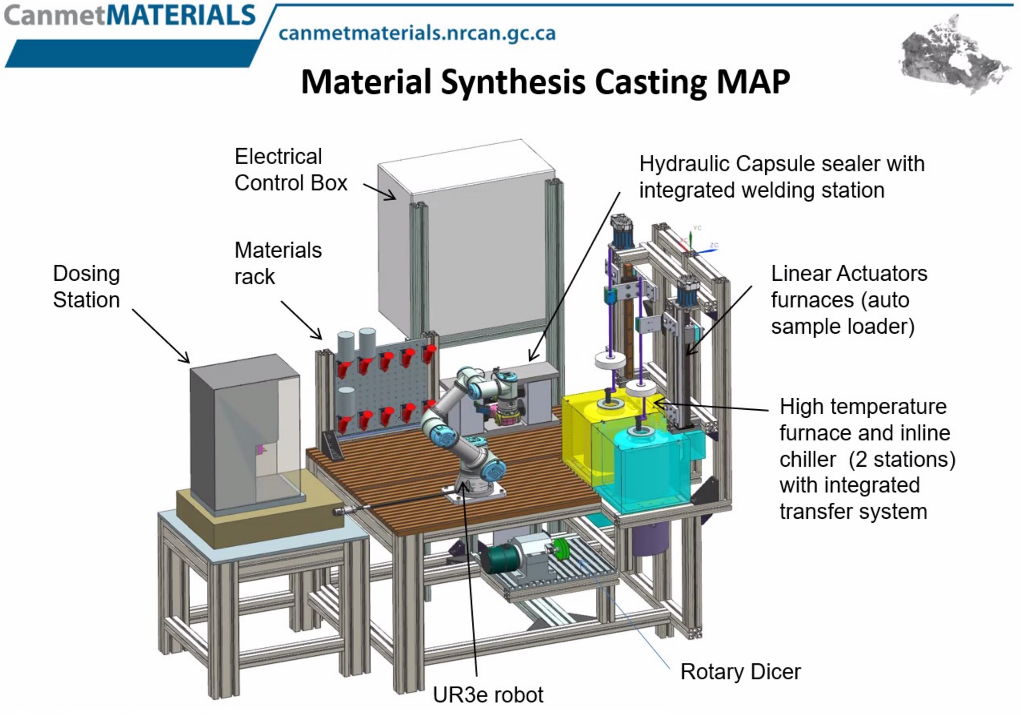
Find optimal electrolyte

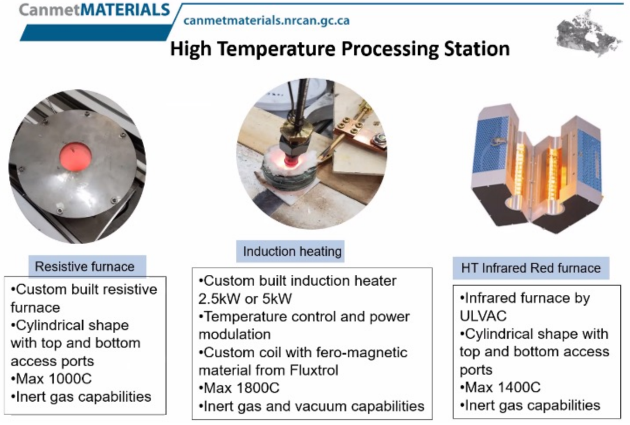
- $\max(conductivity)$
- $\max(redox\ potential)$
- $pH = 7.5$
- $\min(costs)$

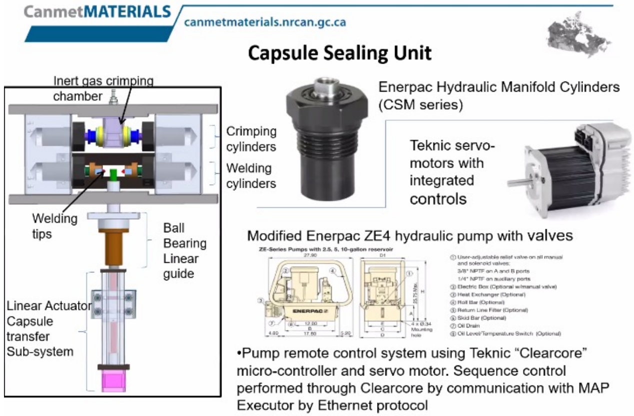


Source: https://www.youtube.com/watch?v=SX26XRFx0U0

Autonomous materials development platforms

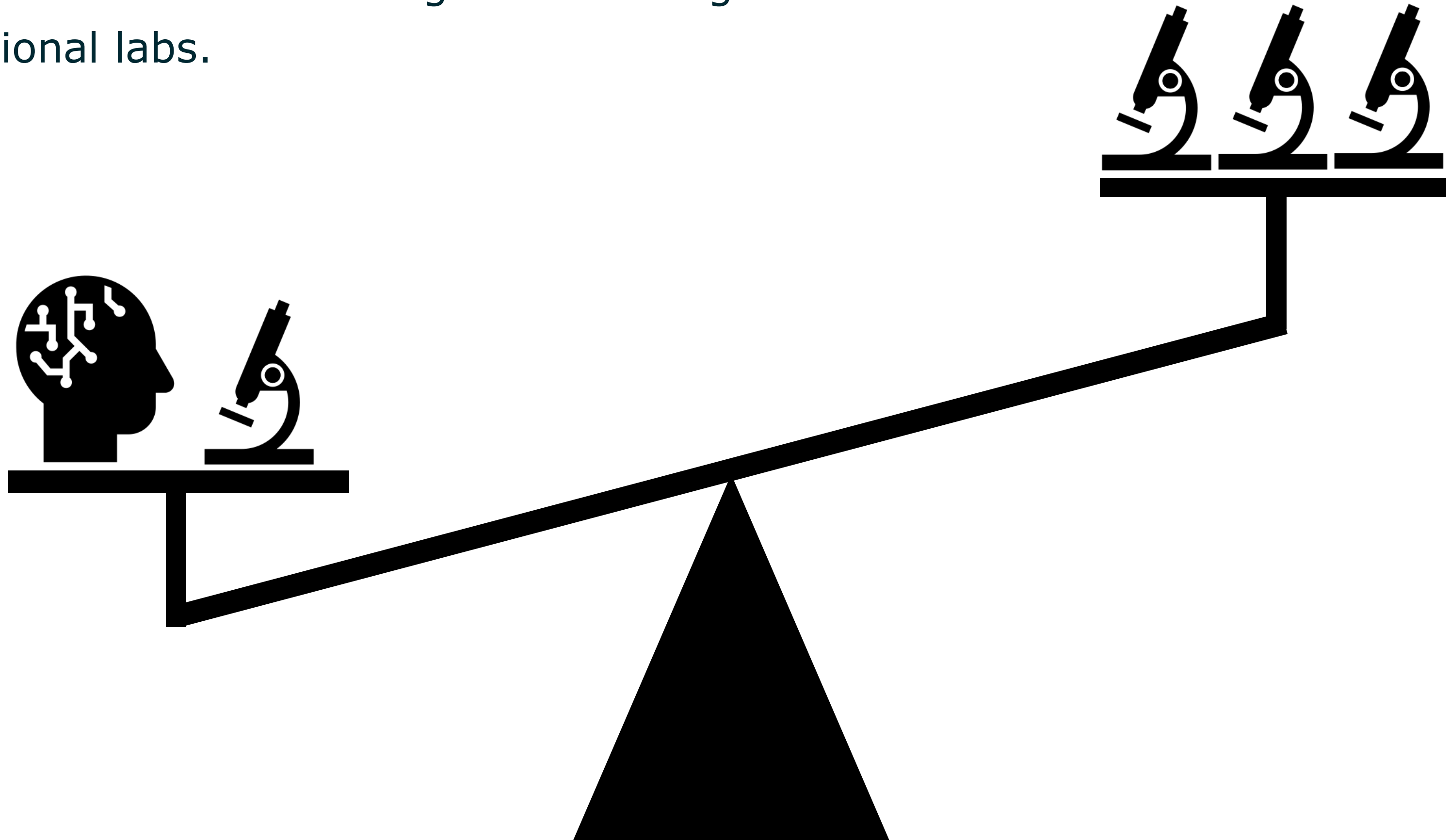






GCMAC User Workshop, presentation of Gabriel Birsan
CanmetMATERIALS, Hamilton, CA

Data-driven labs “out-weight” much larger traditional labs.



Bonus Material:

SLAMD - an AI app for inverse design

www.bam.de

SLAMD Dashboard Home Base Blend Formulations Discovery ?

BAM

SLAMD - Sequential Learning App for Materials Discovery

Leverage the Digital Lab and AI optimization to discover exciting new concrete recipes

> Represent resources and processes and their socio-economic impact.
> Calculate complex compositions and enrich them with detailed material knowledge.
> Integrate laboratory data and apply it to novel formulations.
> Tailor concretes to the purpose to achieve the best solution.

Workflow

1. Digital Lab

1. Specify resources
From base materials to manufacturing processes – "Base" enables a detailed and consistent description of existing resources.

2. Combine resources
The combination of base materials and processes offers an almost infinite optimization potential. "Blending" makes it easier to design complex configurations.

3. Digital recipes
With "Formulations" you can effortlessly convert your resources into the entire spectrum of possible concrete formulations. This automatically generates a detailed set of data for AI optimization.

2. AI-Optimization

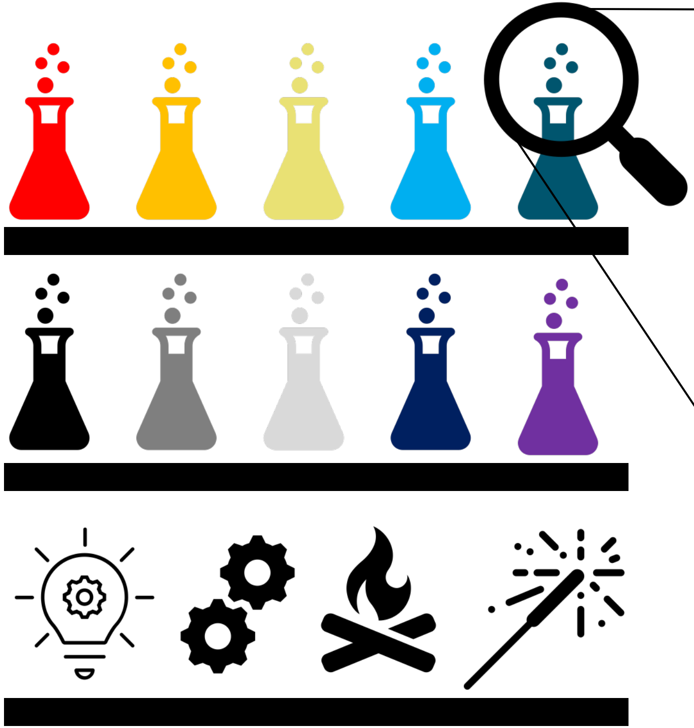
4. Materials Discovery
Integrate data from the "Digital Lab" or upload your own material data. Enrich the data with lab results and adopt the knowledge to new recipes via artificial intelligence. Leverage socio-economic metrics to identify recipes tailored to your requirements.

Link:
github.com/BAMresearch/WEBSLAMD

Links

GitHub Repository | BAM website | User Manual | Powered by iteratec

Digital Lab



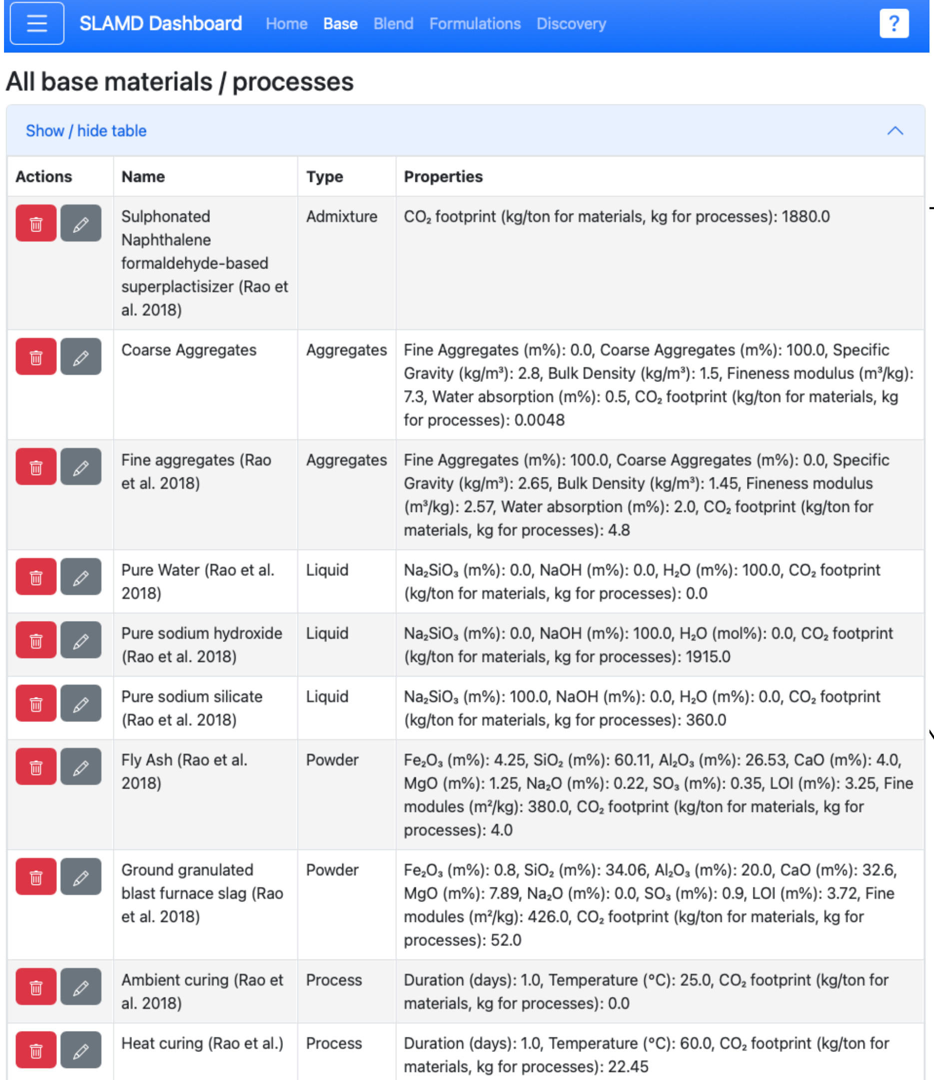
Digital Twin

Materials prop.

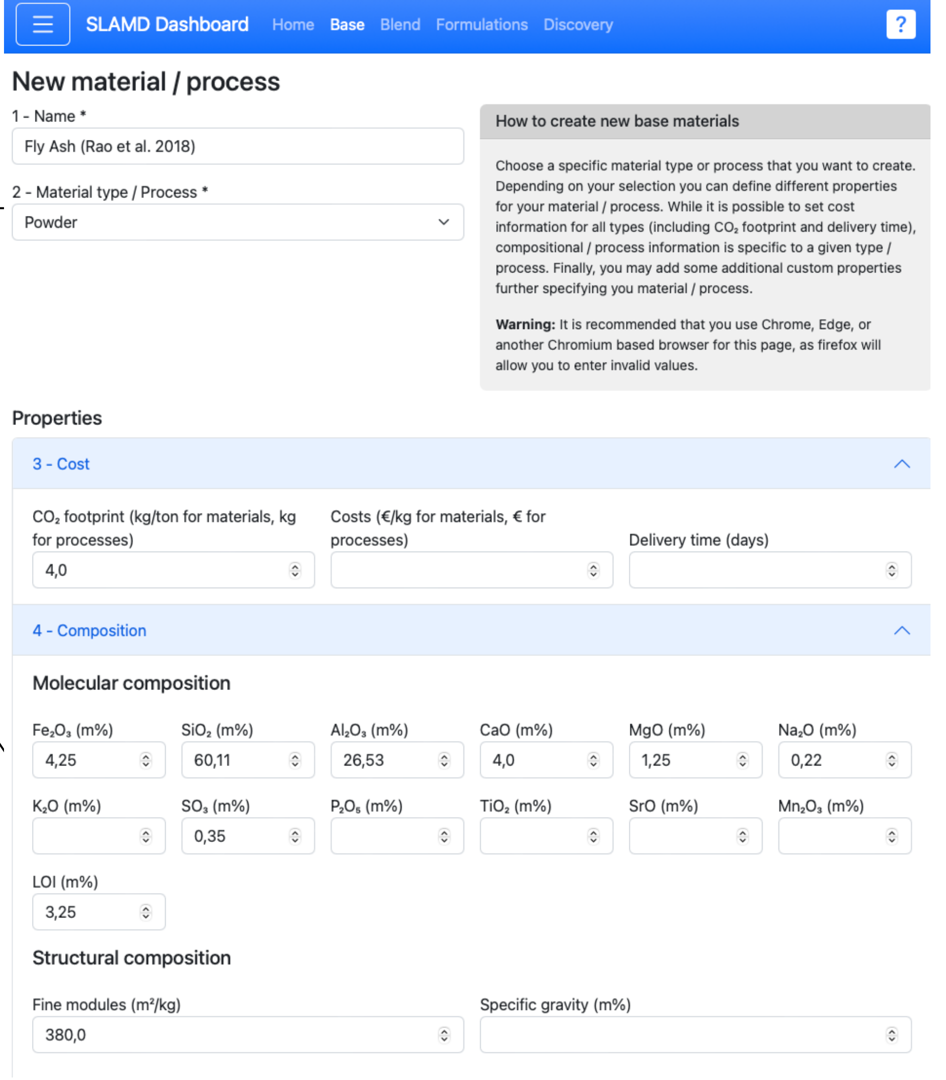
- ………$\% \, CaO$
- ……… $\% \, SiO_2$
- ……… mm^2/g
- ………

Socio-eco. prop.

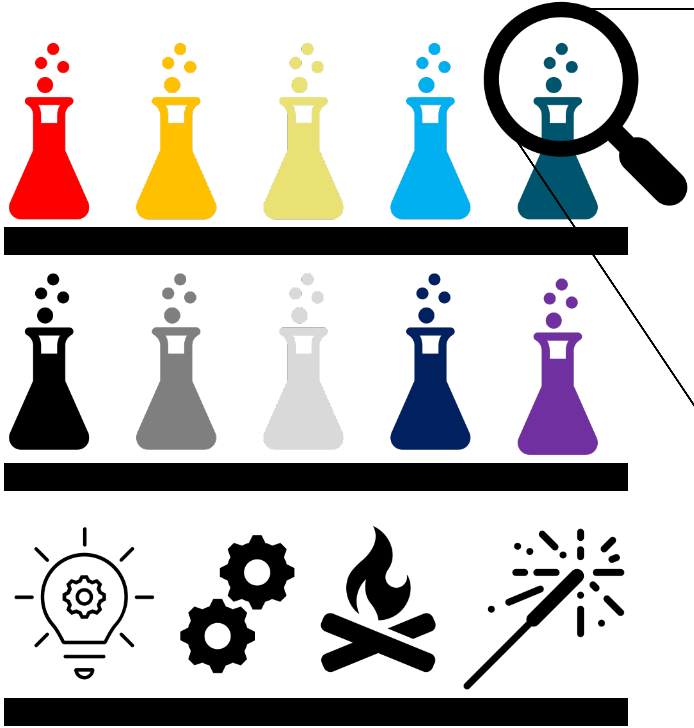
- ……… $kgCO_2$
- ……… €
- ……… %



Actions	Name	Type	Properties
	Sulphonated Naphthalene formaldehyde-based superplacticizer (Rao et al. 2018)	Admixture	CO_2 footprint (kg/ton for materials, kg for processes): 1880.0
	Coarse Aggregates	Aggregates	Fine Aggregates (m%): 0.0, Coarse Aggregates (m%): 100.0, Specific Gravity (kg/m³): 2.8, Bulk Density (kg/m³): 1.5, Fineness modulus (m³/kg): 7.3, Water absorption (m%): 0.5, CO_2 footprint (kg/ton for materials, kg for processes): 0.0048
	Fine aggregates (Rao et al. 2018)	Aggregates	Fine Aggregates (m%): 100.0, Coarse Aggregates (m%): 0.0, Specific Gravity (kg/m³): 2.65, Bulk Density (kg/m³): 1.45, Fineness modulus (m³/kg): 2.57, Water absorption (m%): 2.0, CO_2 footprint (kg/ton for materials, kg for processes): 4.8
	Pure Water (Rao et al. 2018)	Liquid	Na_2SiO_3 (m%): 0.0, NaOH (m%): 0.0, H_2O (m%): 100.0, CO_2 footprint (kg/ton for materials, kg for processes): 0.0
	Pure sodium hydroxide (Rao et al. 2018)	Liquid	Na_2SiO_3 (m%): 0.0, NaOH (m%): 100.0, H_2O (mol%): 0.0, CO_2 footprint (kg/ton for materials, kg for processes): 1915.0
	Pure sodium silicate (Rao et al. 2018)	Liquid	Na_2SiO_3 (m%): 100.0, NaOH (m%): 0.0, H_2O (m%): 0.0, CO_2 footprint (kg/ton for materials, kg for processes): 360.0
	Fly Ash (Rao et al. 2018)	Powder	Fe_2O_3 (m%): 4.25, SiO_2 (m%): 60.11, Al_2O_3 (m%): 26.53, CaO (m%): 4.0, MgO (m%): 1.25, Na_2O (m%): 0.22, SO_3 (m%): 0.35, LOI (m%): 3.25, Fine modules (m²/kg): 380.0, CO_2 footprint (kg/ton for materials, kg for processes): 4.0
	Ground granulated blast furnace slag (Rao et al. 2018)	Powder	Fe_2O_3 (m%): 0.8, SiO_2 (m%): 34.06, Al_2O_3 (m%): 20.0, CaO (m%): 32.6, MgO (m%): 7.89, Na_2O (m%): 0.0, SO_3 (m%): 0.9, LOI (m%): 3.72, Fine modules (m²/kg): 426.0, CO_2 footprint (kg/ton for materials, kg for processes): 52.0
	Ambient curing (Rao et al. 2018)	Process	Duration (days): 1.0, Temperature (°C): 25.0, CO_2 footprint (kg/ton for materials, kg for processes): 0.0
	Heat curing (Rao et al.)	Process	Duration (days): 1.0, Temperature (°C): 60.0, CO_2 footprint (kg/ton for materials, kg for processes): 22.45



Digital Lab



Digital Twin

👩‍🔬 Materials prop.

🧪 ....% CaO

.... % SiO_2

🔎 .... mm^2/g

🎨 ....

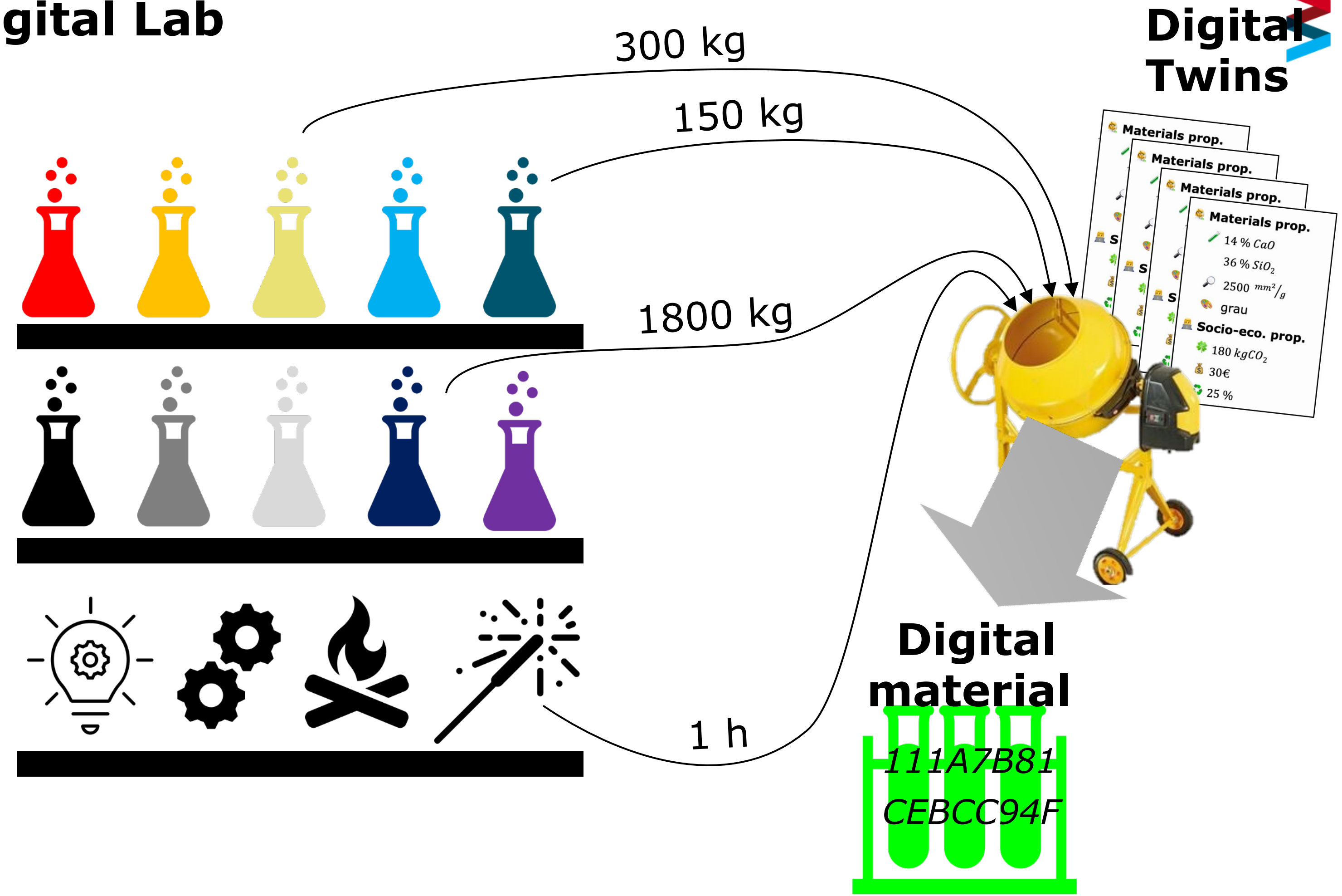
👨‍💻 Socio-eco. prop.

🍀 .... $kgCO_2$

💰 .... €

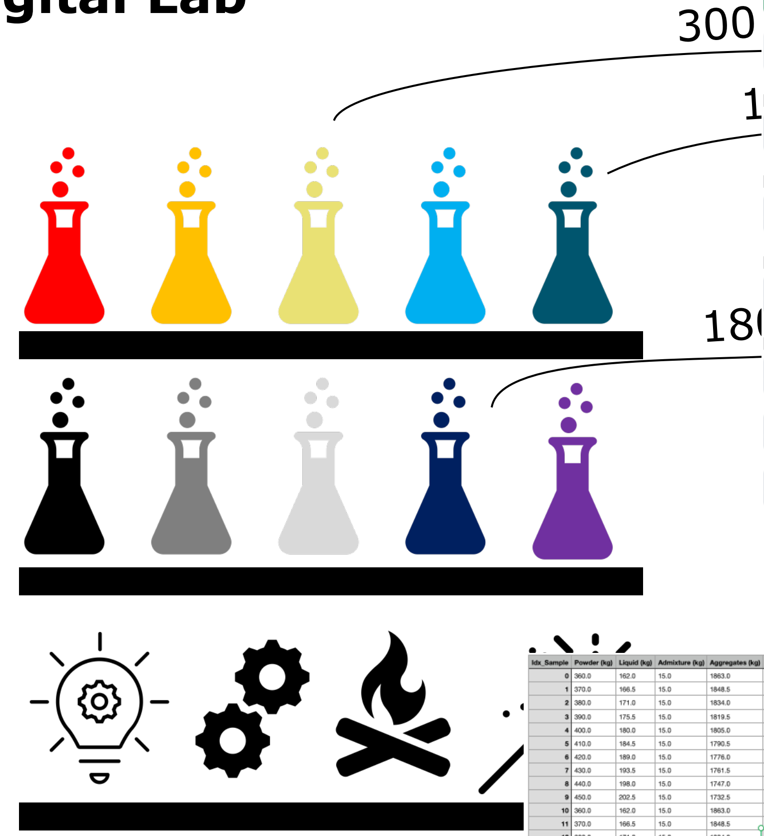
♻️ .... %

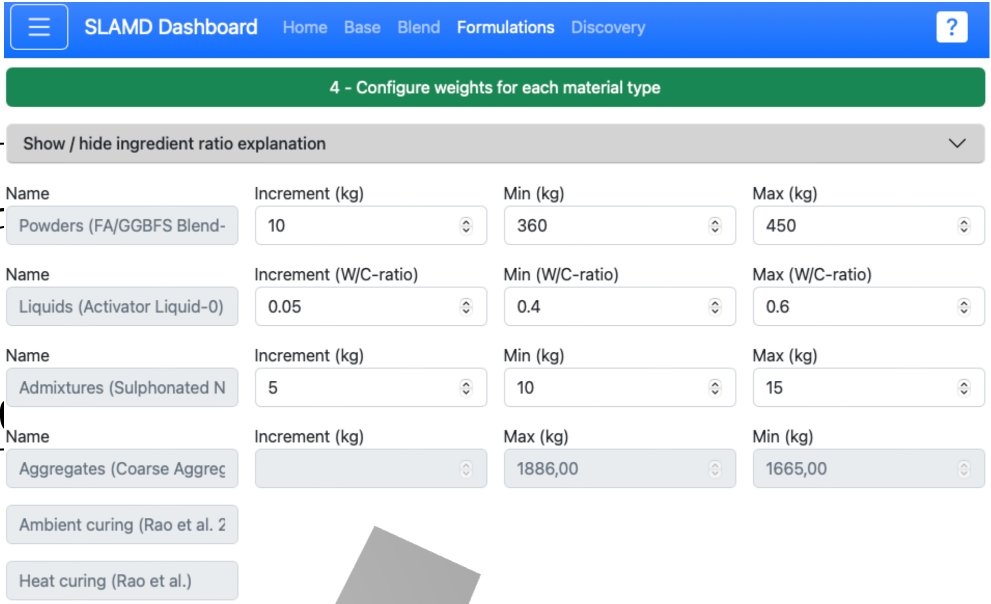
Digital Lab

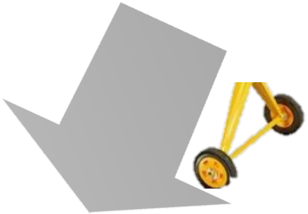


300 kg
150 kg
1800 kg
1 h
Digital Twins
Materials prop.
14 % CaO
36 % SiO_2
2500 mm^2/g
grau
Socio-eco. prop.
180 $kgCO_2$
30€
25 %
Digital material
111A7B81
CEBCC94F

Digital Lab



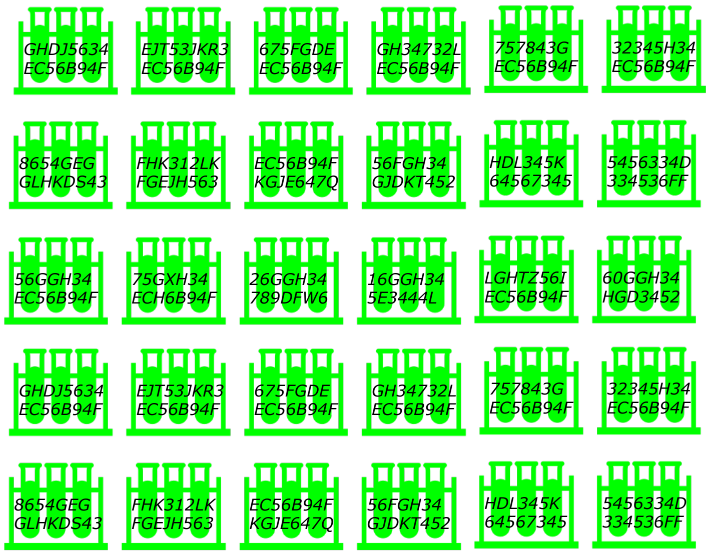




Idx_Sample	Powder (kg)	Liquid (kg)	Admixture (kg)	Aggregates (kg)	Materials	fe3_o2	al2_o3	ca_o	mg_o	s_o3	loi	fine	gravity	na2_si_o3	na_o_h	fine_aggregates	coarse_aggregates	bulk_density
0	360.0	162.0	15.0	1863.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
1	370.0	166.5	15.0	1848.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
2	380.0	171.0	15.0	1834.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
3	390.0	175.5	15.0	1819.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
4	400.0	180.0	15.0	1805.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
5	410.0	184.5	15.0	1790.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
6	420.0	189.0	15.0	1776.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
7	430.0	193.5	15.0	1761.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
8	440.0	198.0	15.0	1747.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
9	450.0	202.5	15.0	1732.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
10	360.0	162.0	15.0	1863.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
11	370.0	166.5	15.0	1848.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
12	380.0	171.0	15.0	1834.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
13	390.0	175.5	15.0	1819.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
14	400.0	180.0	15.0	1805.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
15	410.0	184.5	15.0	1790.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
16	420.0	189.0	15.0	1776.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
17	430.0	193.5	15.0	1761.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
18	440.0	198.0	15.0	1747.0	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
19	450.0	202.5	15.0	1732.5	FA/GGBFS Blend-0.5/0.5, Activator Liquid-0, Sulphonated N	2.52	23.27	18.3	4.57	0.62	3.49	403.0	2.74	30.0	11.5	40.0	60.0	1.48
20	360.0	162.0	15.0	1863.0	FA/GGBFS Blend-0.6/0.4, Activator Liquid-0, Sulphonated N	2.87	23.92	15.44	3.91	0.57	3.44	398.4	2.74	30.0	11.5	40.0	60.0	1.48
21	370.0	166.5	15.0	1848.5	FA/GGBFS Blend-0.6/0.4, Activator Liquid-0, Sulphonated N	2.87	23.92	15.44	3.91	0.57	3.44	398.4	2.74	30.0	11.5	40.0	60.0	1.48
22	380.0	171.0	15.0	1834.0	FA/GGBFS Blend-0.6/0.4, Activator Liquid-0, Sulphonated N	2.87	23.92	15.44	3.91	0.57	3.44	398.4	2.74	30.0	11.5	40.0	60.0	1.48
23	390.0	175.5	15.0	1819.5	FA/GGBFS Blend-0.6/0.4, Activator Liquid-0, Sulphonated N	2.87	23.92	15.44	3.91	0.57	3.44	398.4	2.74	30.0	11.5	40.0	60.0	1.48

AI Optimization - Materials discovery dashboard

Import materials search space



Set objectives

Strenght (Maximize)
Threshold: 45 MPa

Costs (Minimize)
Threshold: 90 €
CO_2-Footprint (Minimize)
Threshold: 120 kg/ton

SLAMD Dashboard Home Base Blend Formulations **Discovery**

Actions	Name	Columns
	Sample_GroundTruth.csv	['Idx_Sample', 'Powderkg', 'Liquidkg', 'WC', 'Admixturekg', 'Aggregateskg', 'Materials', 'fe3_o2', 'al2_o3', 'ca_o', 'mg_o', 's_o3', 'loi', 'fine', 'gravity', 'na2_si_o3', 'na_o_h', 'fine_aggregates', 'coarse_aggregates', 'bulk_density', 'fineness_modulus', 'water_absorption', 'duration', 'temperature', 'totalCostsTon', 'totalCo2_footprintTon', 'totalDelivery_time', 'fc_28dGroundTruth', 'fc_28dPredicted']

Show / hide materials discovery explanation

Materials Data (Input) (select one column at least)

fe3_o2
al2_o3
ca_o
mg_o
s_o3
loi
fine
gravity

Target Properties (select one column at least)

Idx_Sample
totalCostsTon
totalCo2_footprintTon
totalDelivery_time
fc_28dGroundTruth
fc_28dPredicted

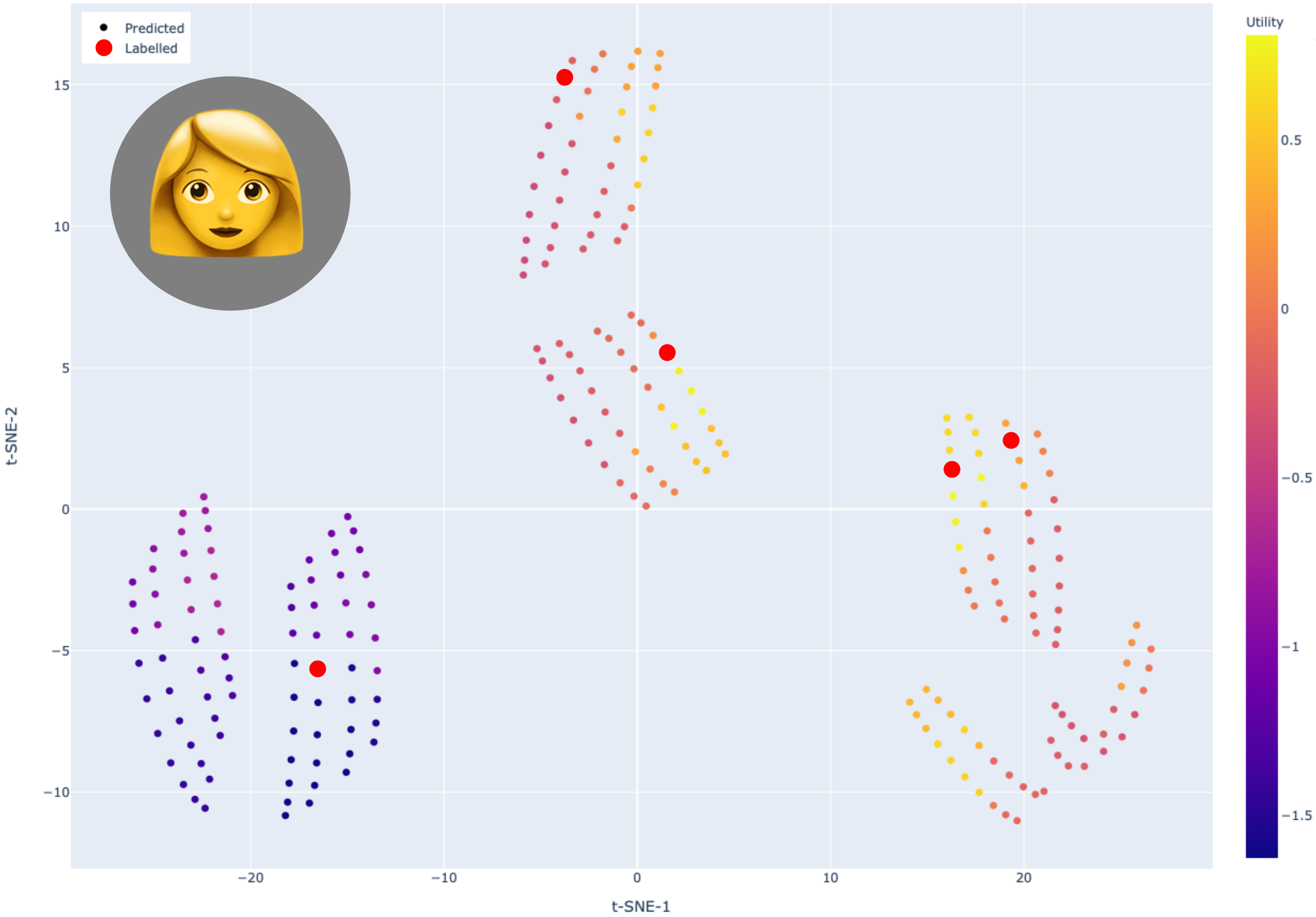
A priori Information (optional)

Idx_Sample
totalCostsTon
totalCo2_footprintTon
totalDelivery_time
fc_28dGroundTruth

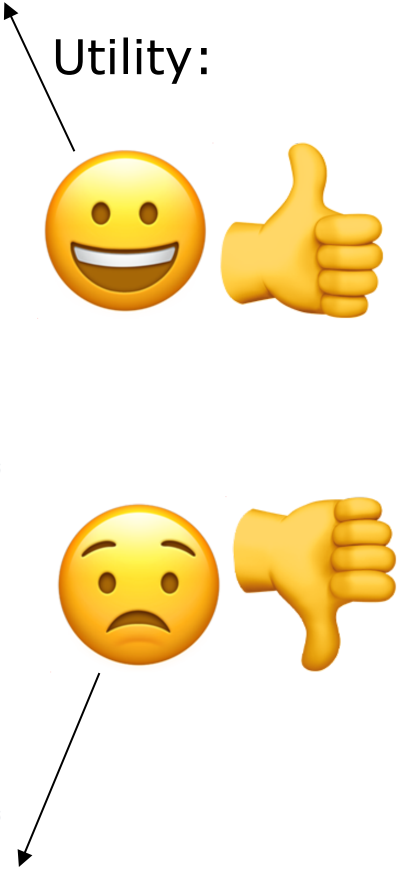
import materials search space

fc_28dPredicted	◉ Maximize	○ Minimize	Weight	1,00	Threshold	45
totalCostsTon	○ Maximize	◉ Minimize	Weight	1,00	Threshold	90
totalCo2_footprintTon	○ Maximize	◉ Minimize	Weight	1,00	Threshold	120
totalDelivery_time	○ Maximize	◉ Minimize	Weight	1,00	Threshold	5

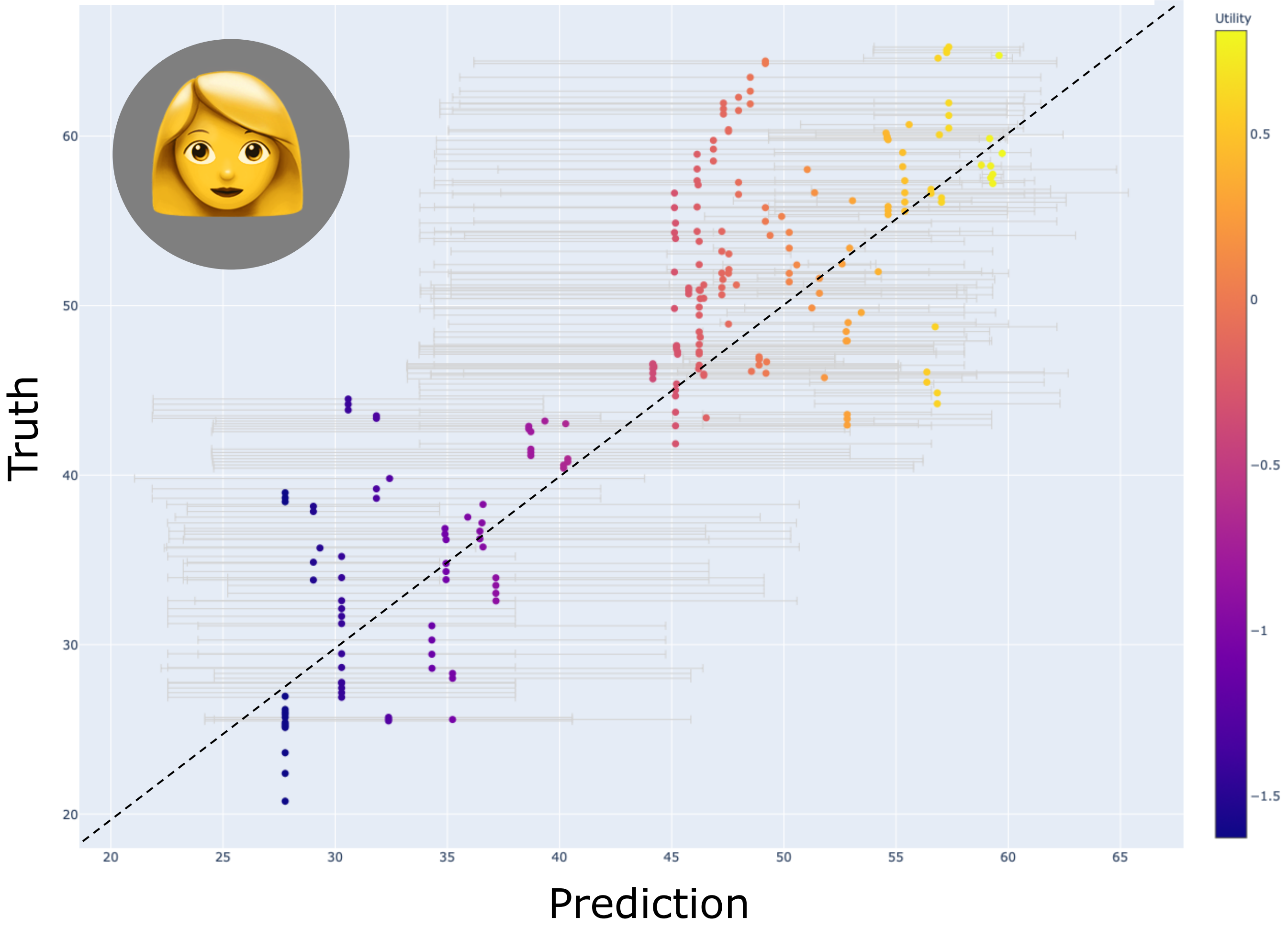
Material search space



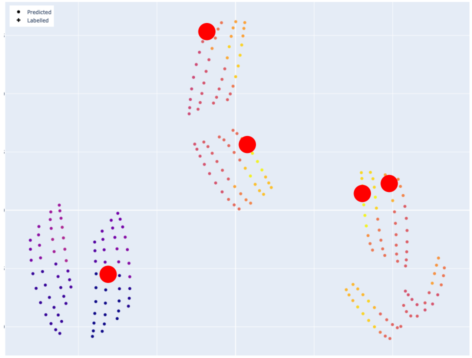
Utility:



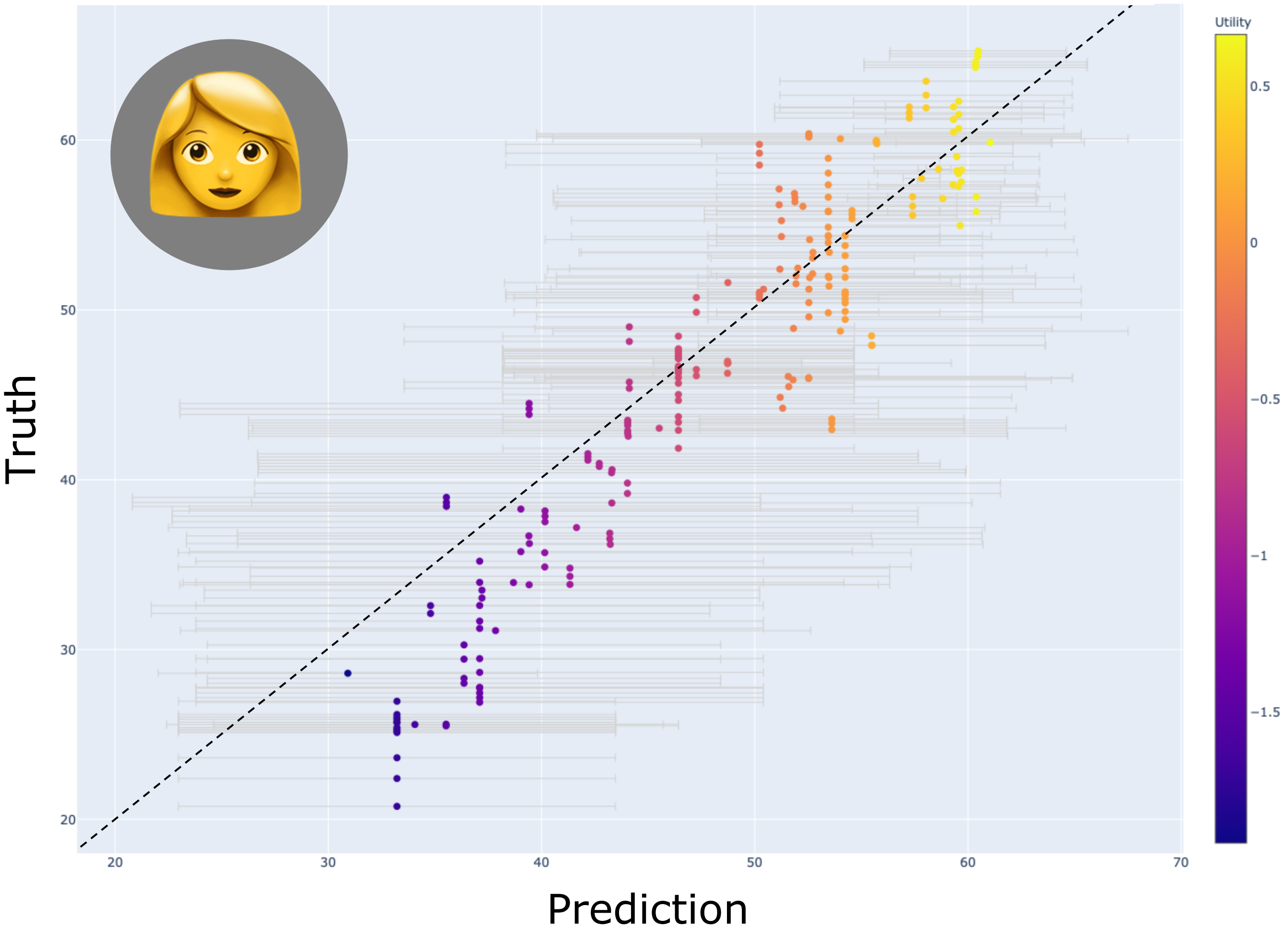
Predicted vs. real target



Training-set size: 5



Predicted vs. real target



Training-set size: 8