AI in Glass Strengthening

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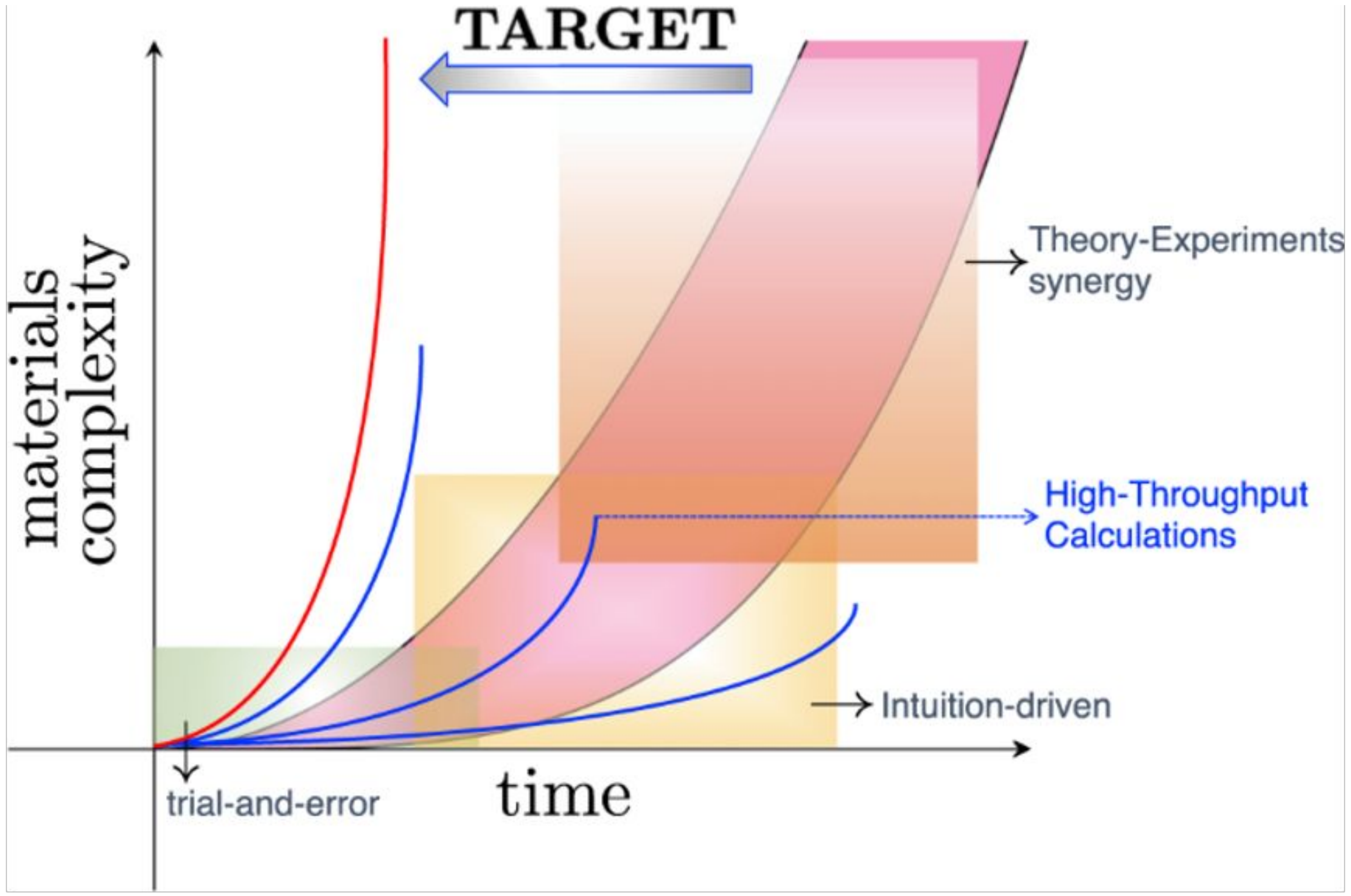
Glass Discovery
Motivation

- Glasses: back-bone of society
- Glass discovery: empirical, uneconomical with a ***design-to-deploy period of 20-30 years***
- UN sustainable development goals: 10/17 can potentially be addressed through glass innovation: IYG
- Areas: energy, infrastructure, healthcare, CO_2 emission, space sector



Lookman et al., npj Comp. Mat., 2019

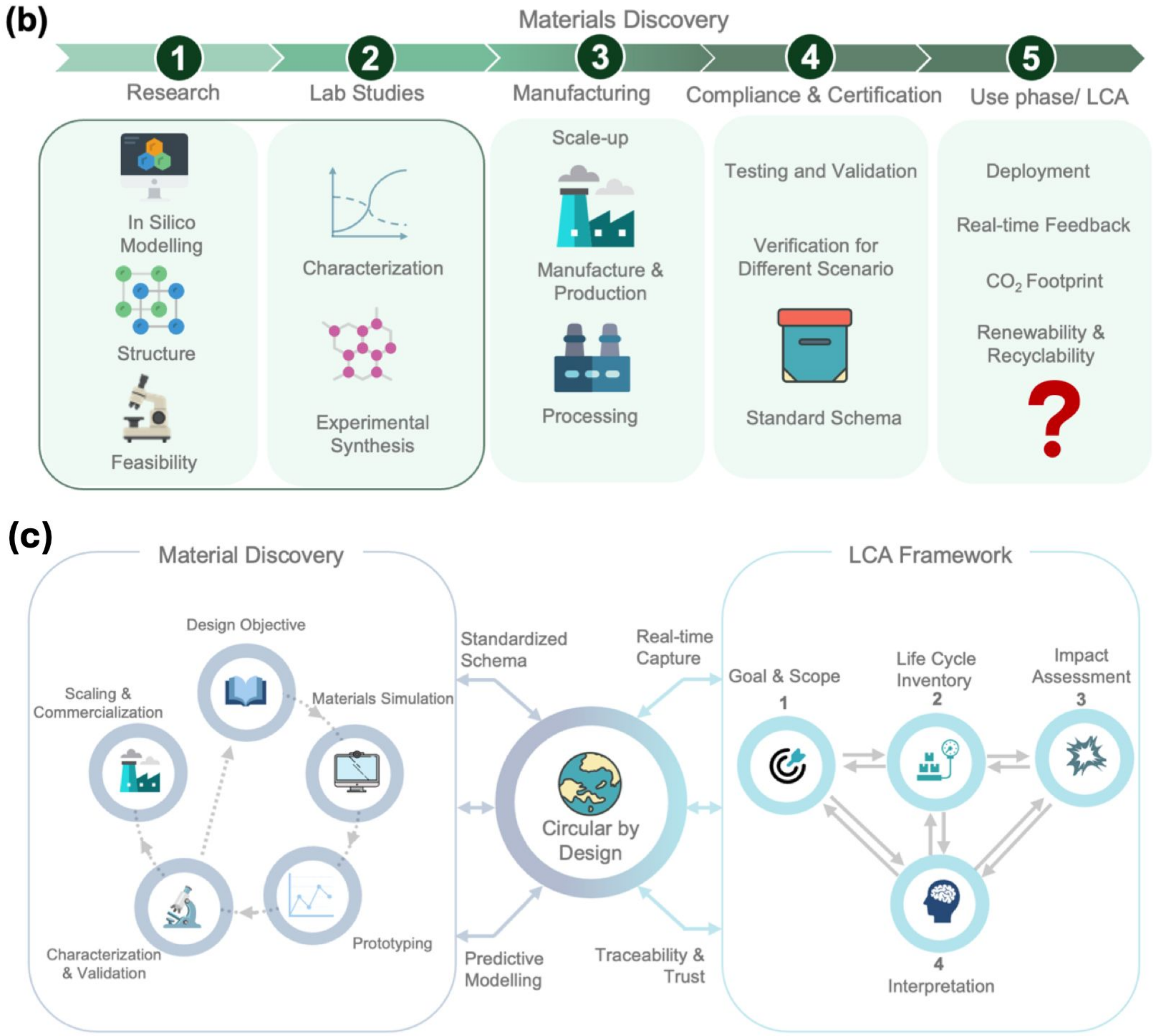
Alternate approach: Data-driven Modeling

AI Scientist for Glass Discovery

Sustainable Materials Discovery in the Era of Artificial Intelligence

Sajid Mannan[1], Rupert J. Myers[2], Rohit Batra[3], Rocio Mercado[4], Lothar Wondraczek[5,6], N. M. Anoop Krishnan[1,7,*]

Nature Sustainability *(accepted)*



Informatic

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Industrial Scale Manufacturing

AI-driven process optimization at industrial scale

Overtrained Language Models Are Harder to Fine-Tune

Jacob Mitchell Springer[1] Sachin Goyal[1] Kaiyue Wen[2] Tanishq Kumar[3] Xiang Yue[1] Sadhika Malladi[4] Graham Neubig[1] Aditi Raghunathan[1]

Kausik Hira[1], Mohd Zaki[2], Mausam[1,3,#], N. M. Anoop Krishnan[1,2,#]
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Resource Published: 14 July 2026

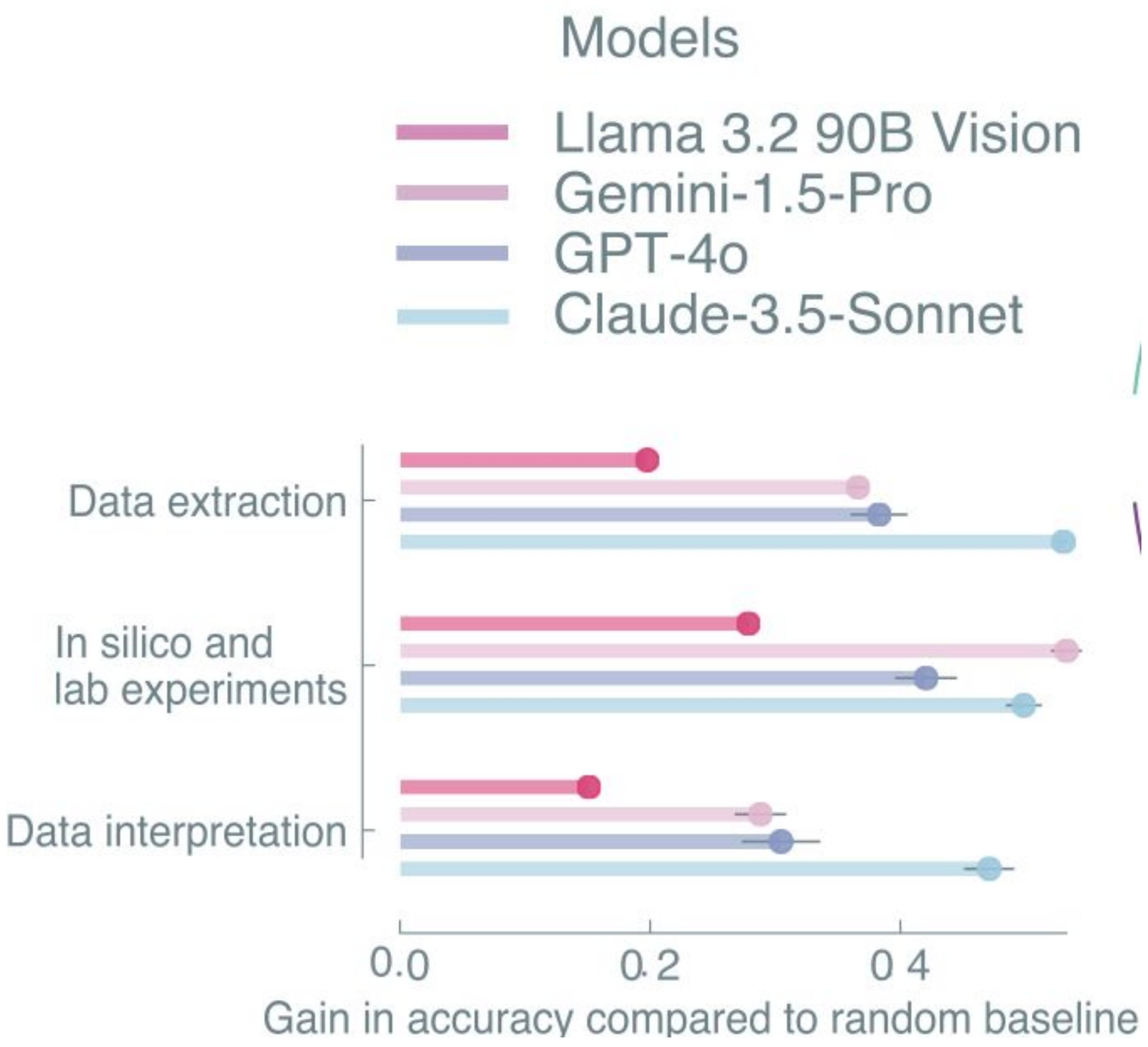
UniFFBench: evaluating universal machine learning force fields against experimental measurements

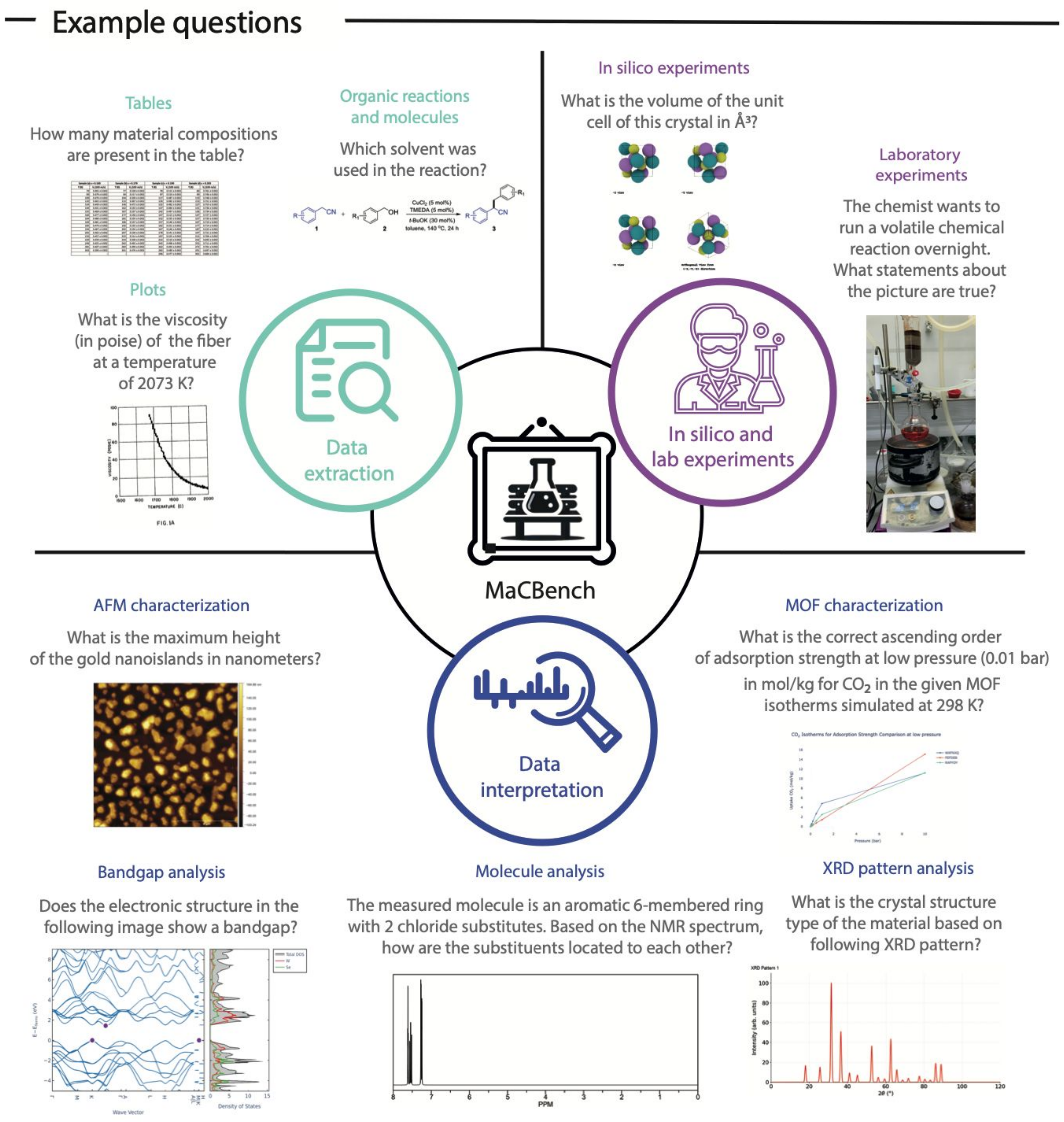
Sajid Mannan, Vaibhav Bihani, Carmelo Gonzales, Kin Long Kelvin Lee, Nitya Nand Gosvami, Sayan Ranu, Santiago Miret & N. M. Anoop Krishnan

Nature Computational Science **6**, 894–906 (2026) | Cite this article

MaCBench

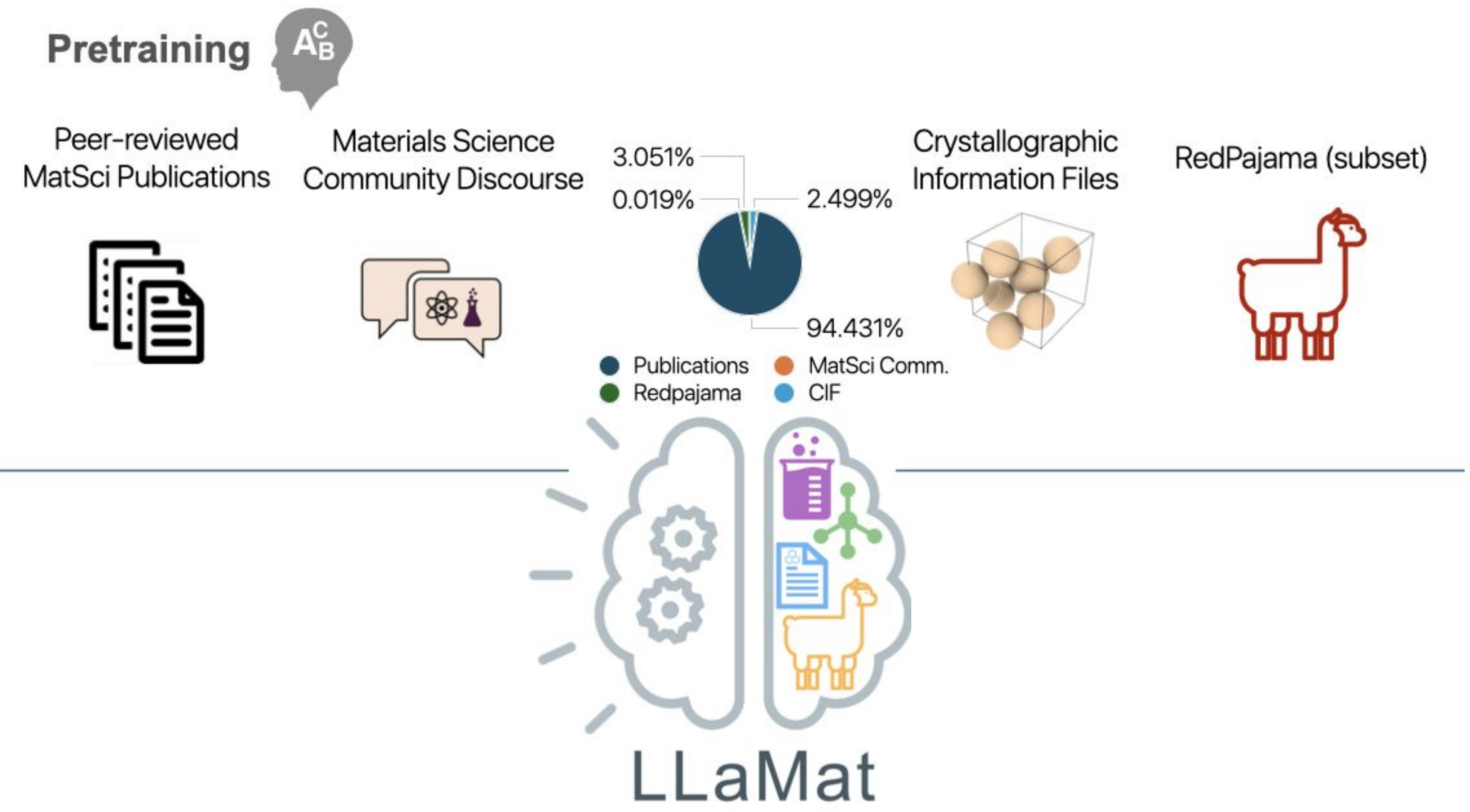
Benchmarking multimodal models

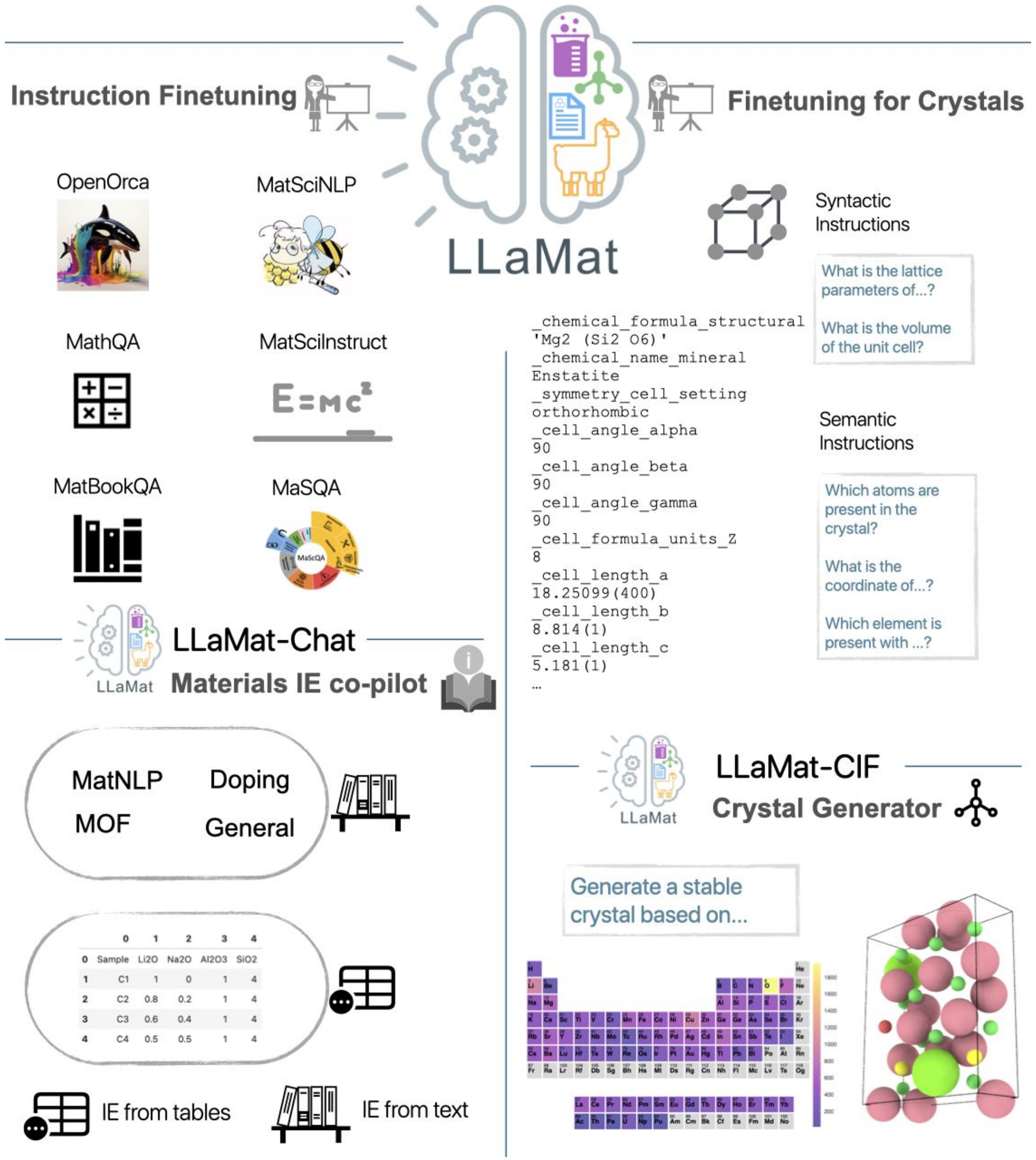




N. Alampara, et al., NMAK, K. Jablonka, Nat. Comput. Sci, 2025

LLaMat
LLM for Materials



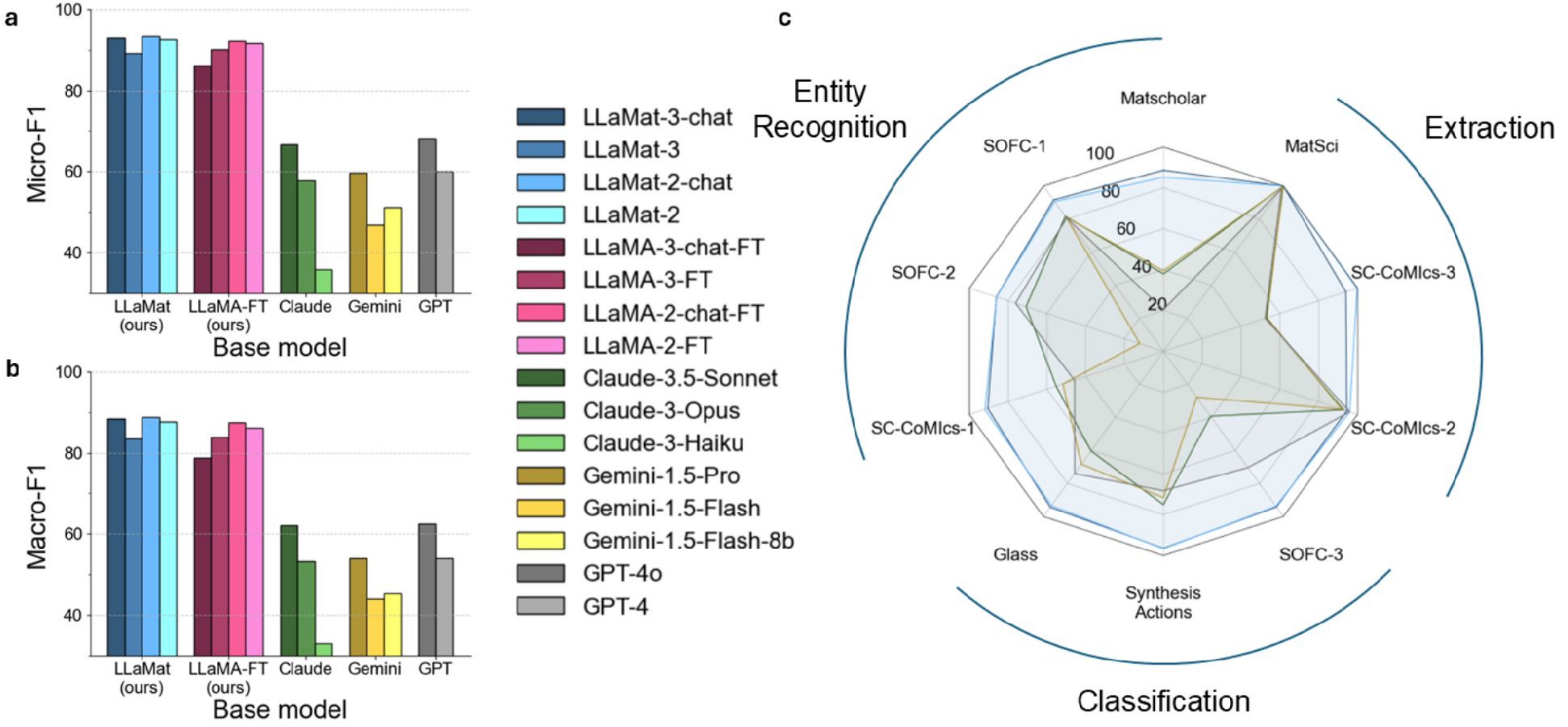


Mishra et al., NMAK Nat. Mach. Intelligence, 2025 (Accepted in principle)

LLaMat

First Large Language Model for Materials

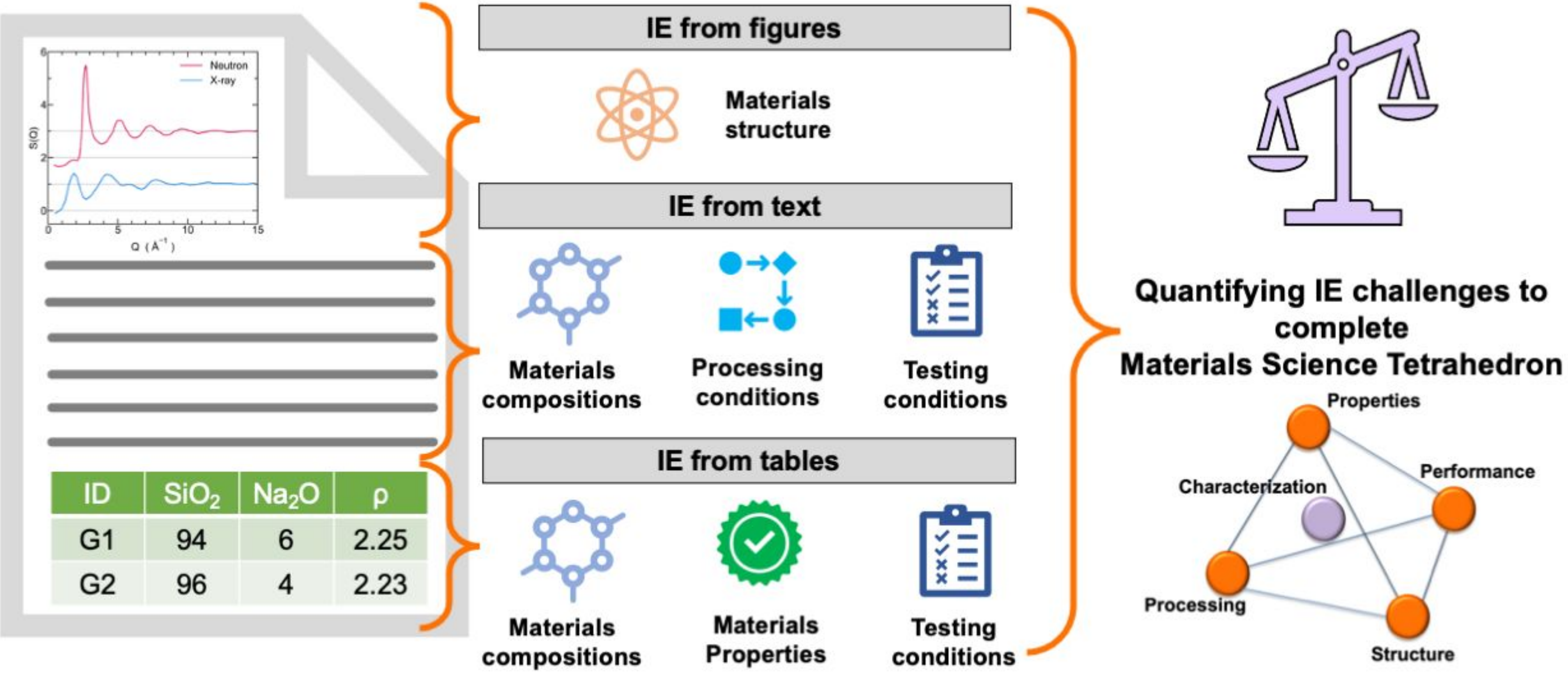
LLaMat significantly outperforms LLMs on MatSci tasks!



Mishra et al., NMAK arXiv, 2024

Information Extraction from Tables

Challenges



Gupta et al., NMAK, Mausam ACL, 2023 Hira et al., NMAK 2023, RSC Digital Discovery

Information Extraction from Tables

Challenges

6. Single-cell compositions: Entire composition in one table cell (some coefficients may be missing)

7. Percentages not summing to 100: Re-normalization is needed. Common case is doping

8. Percentage contributions as variables: Like x, y, etc. Contributions can have arithmetic expressions

9. Partial Info Tables: Percentages of only some constituents reported in table. Infer remaining composition from table caption or publication text

10. Other corner cases

Gupta et al., ACL, 2023

Composition	$\log \sigma_{298}$ (S cm^{-1})
$(80GeS_2–20Ga_2S_3)_{90}–(LiI)_{10}$	−6.34 (5)
$(80GeS_2–20Ga_2S_3)_{90}–(NaCl)_{10}$	−6.92 (5)

Base composition(mol%):$75TeO_2–20ZnO–5Na_2O$

Glass	Tm_2O_3 (wt%)	Yb_2O_3 (wt%)	Ho_2O_3 (wt%)
Undoped TZN	–	–	–
TT05	0.5	–	–
TTY20	1	2	–
TTH05	1	–	0.5
TTYH	1	5	0.15

	$(GeSe_2)_{1-x}(GeBr_4)_x$		$(GeSe_2)_{1-x}Br_x$		
x	0.079	0.167	0.265	0.250	0.429
p_{Sc}(%)	94.1	86.0	76.5	84.1	78.0

Glass composition in the paper:
$20La_2S_3-(80-x)Ga_2S_3-xCsCl$

Glass	CsCl (mol%)	n (1.5 μm)
GLSC10	10	2.253 ± 0.001
GLSC20	20	2.265 ± 0.001

MatSKRAFT

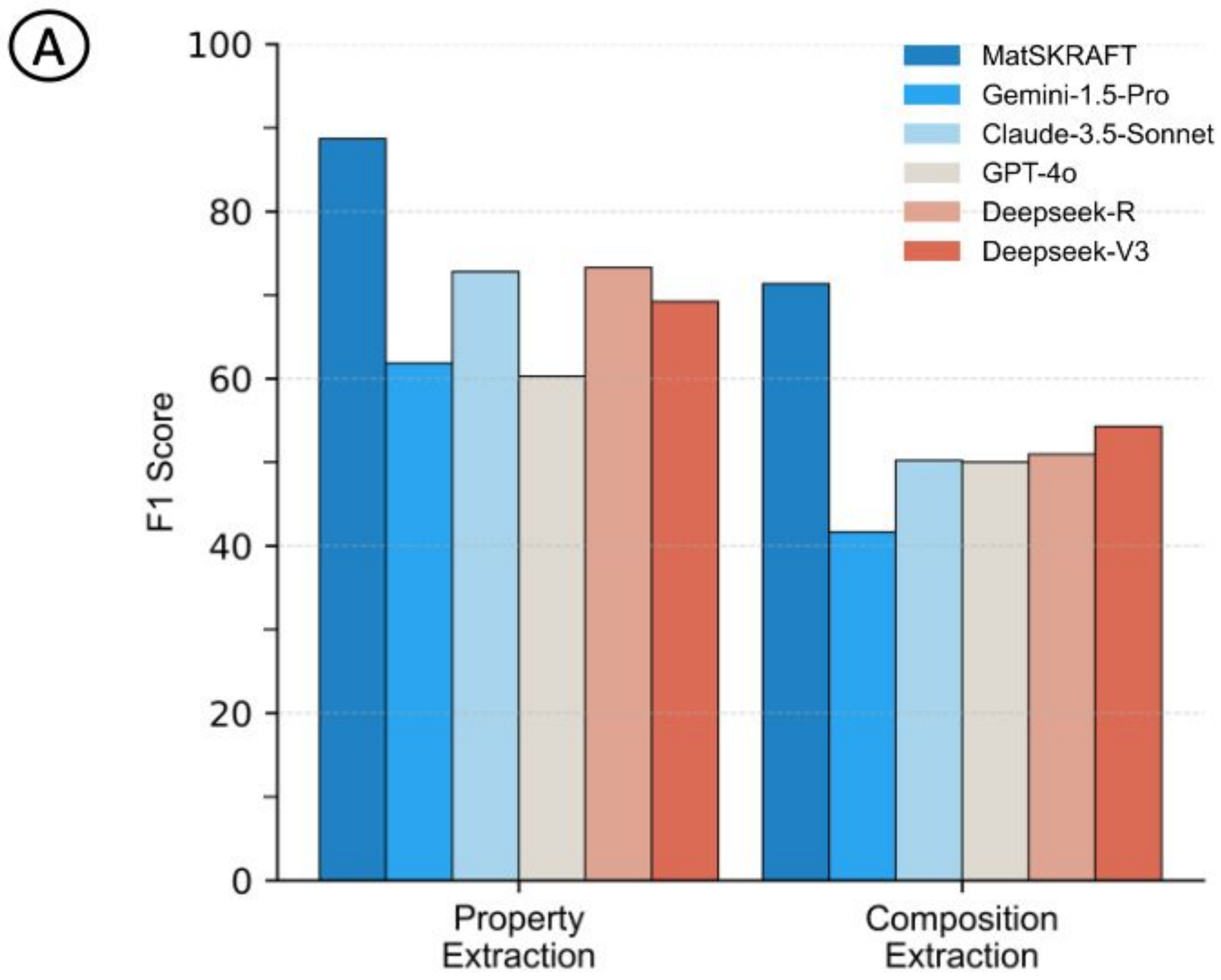
Composition extraction from tables

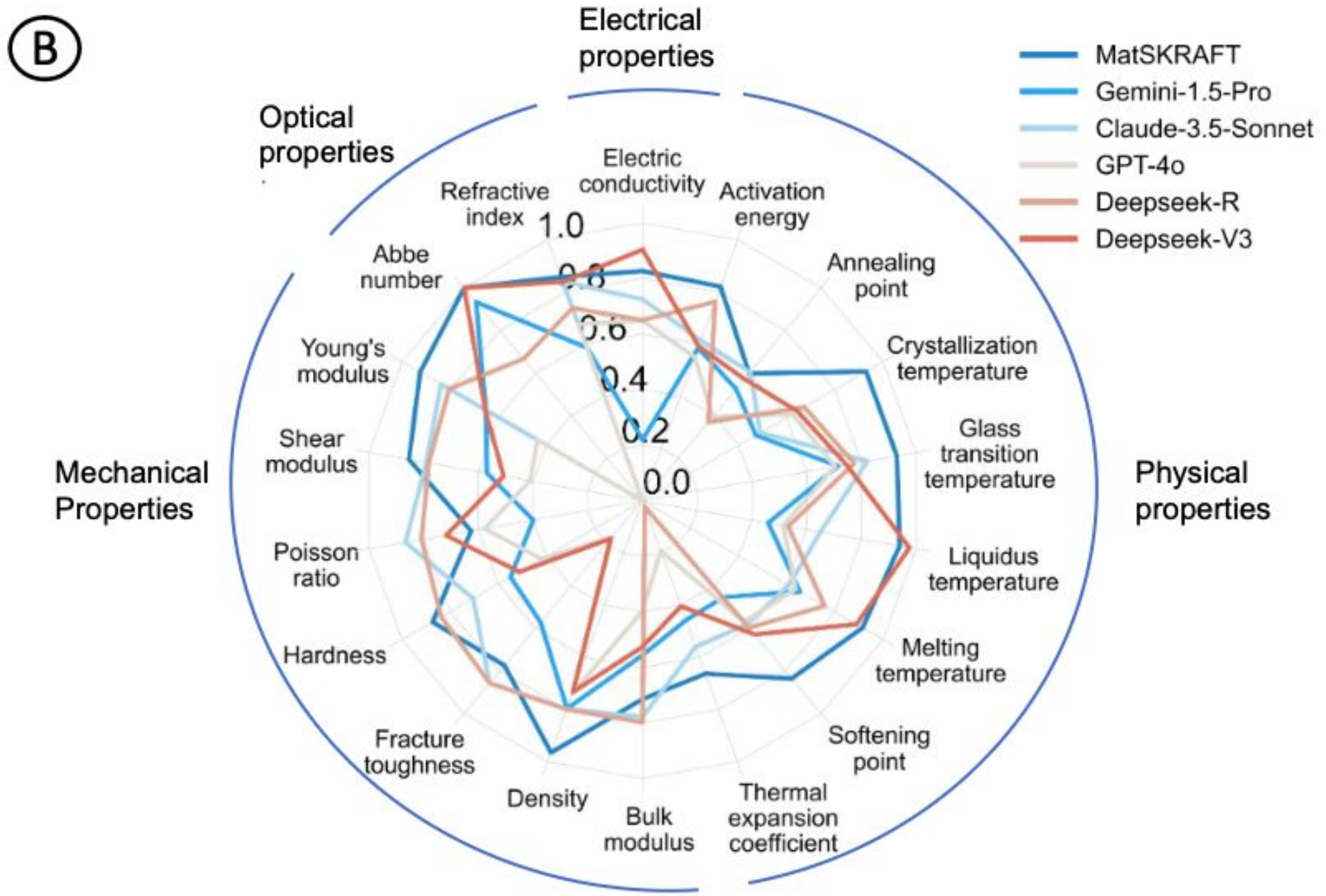
1. Property extraction with units
2. Composition extraction
3. Linking them
4. Applications

Gupta et al., ACM, 2023

MatSKRAFT

Composition and property extraction from tables

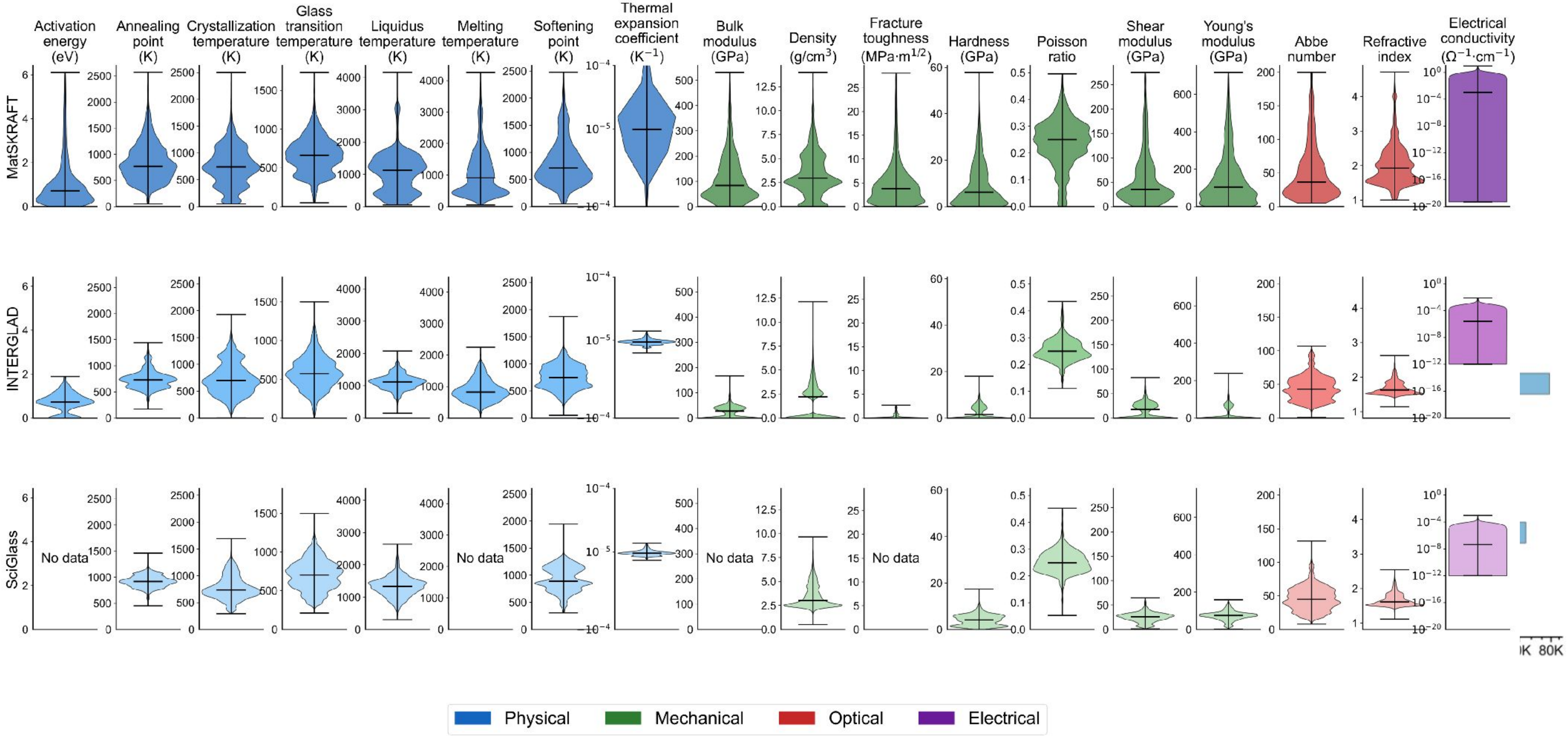




Gupta et al., NMAK, ACL, 2023; Hira et al., NMAK, AI4Mat, NeurIPS, 2024

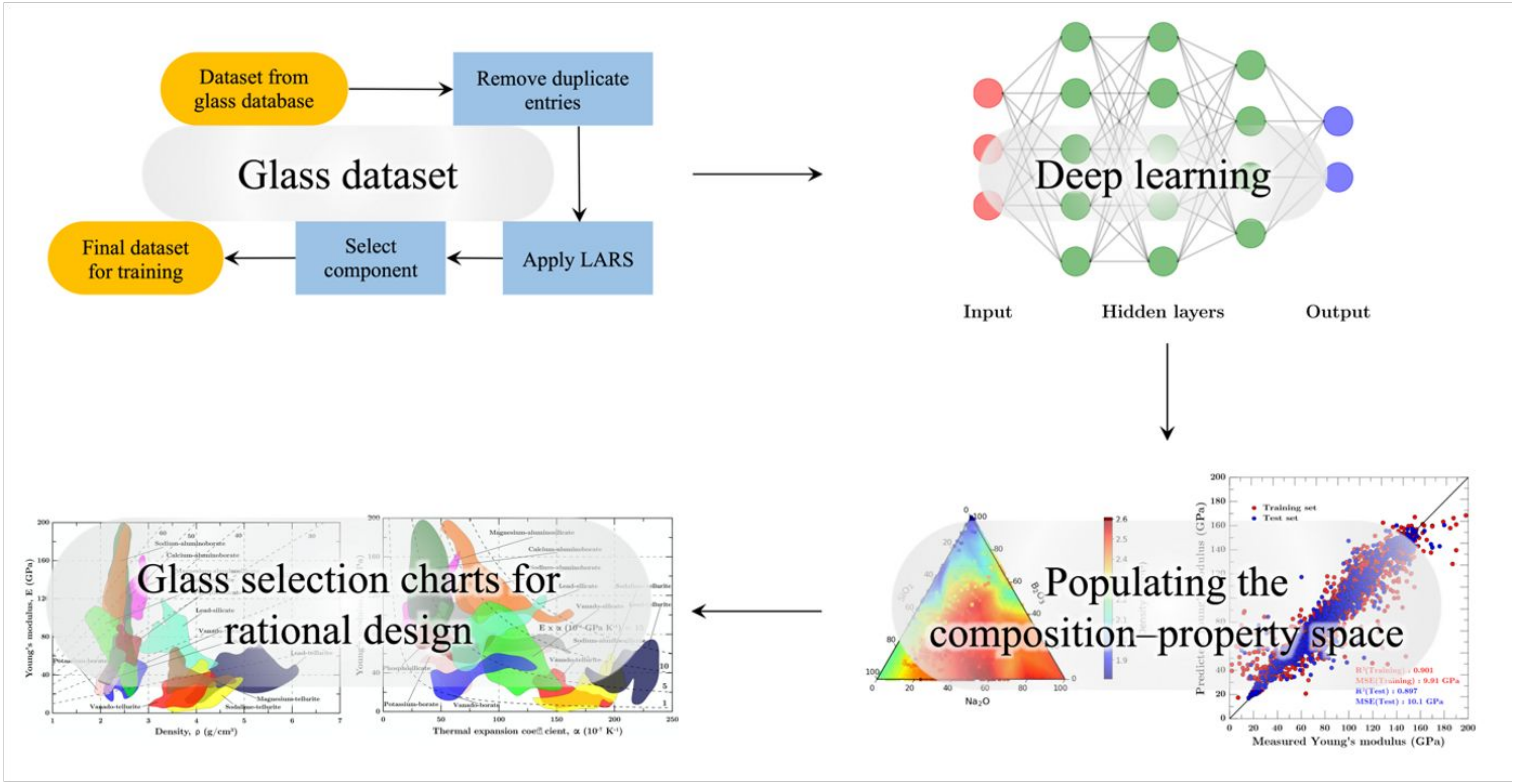
MatSKRAFT

Extracted dataset

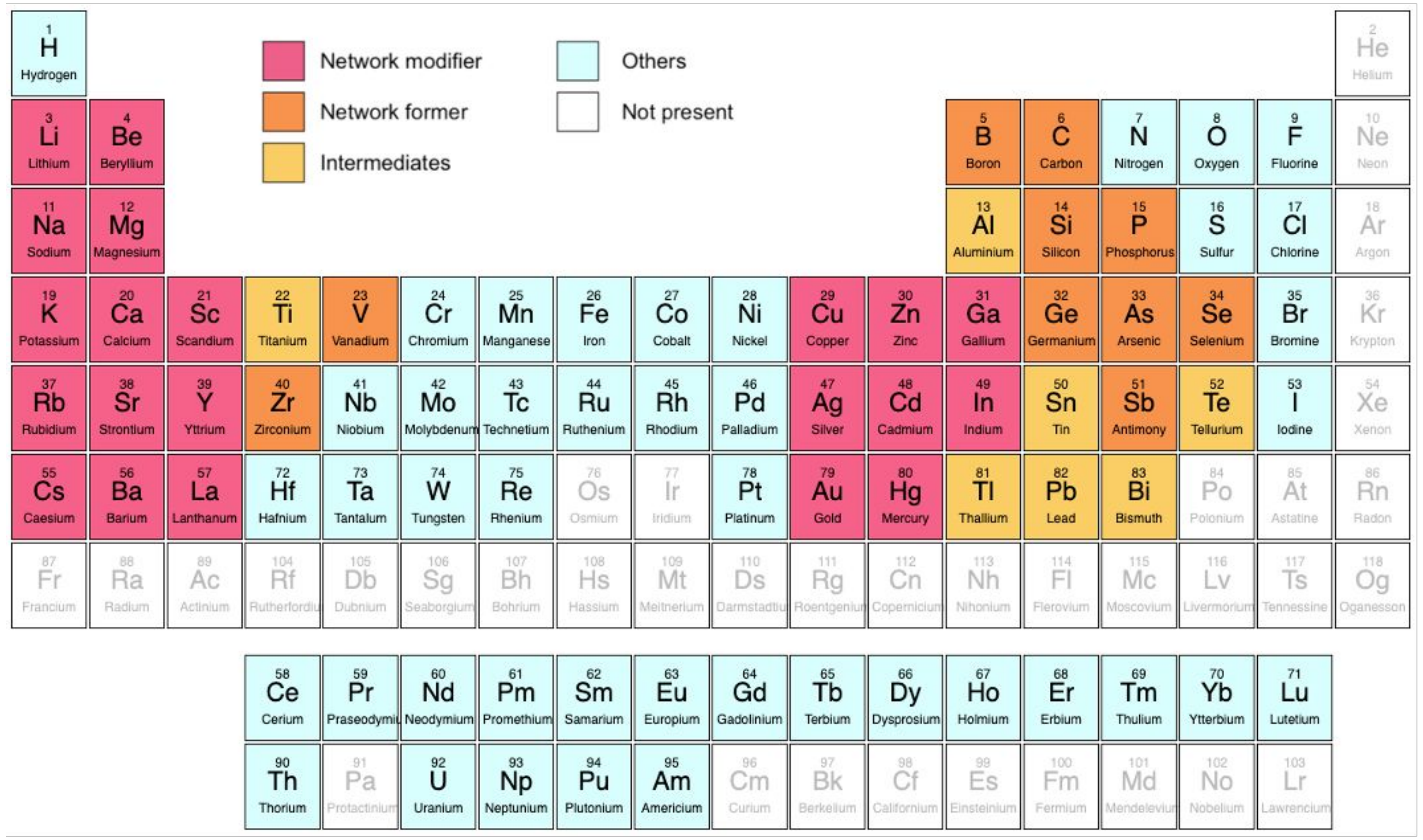


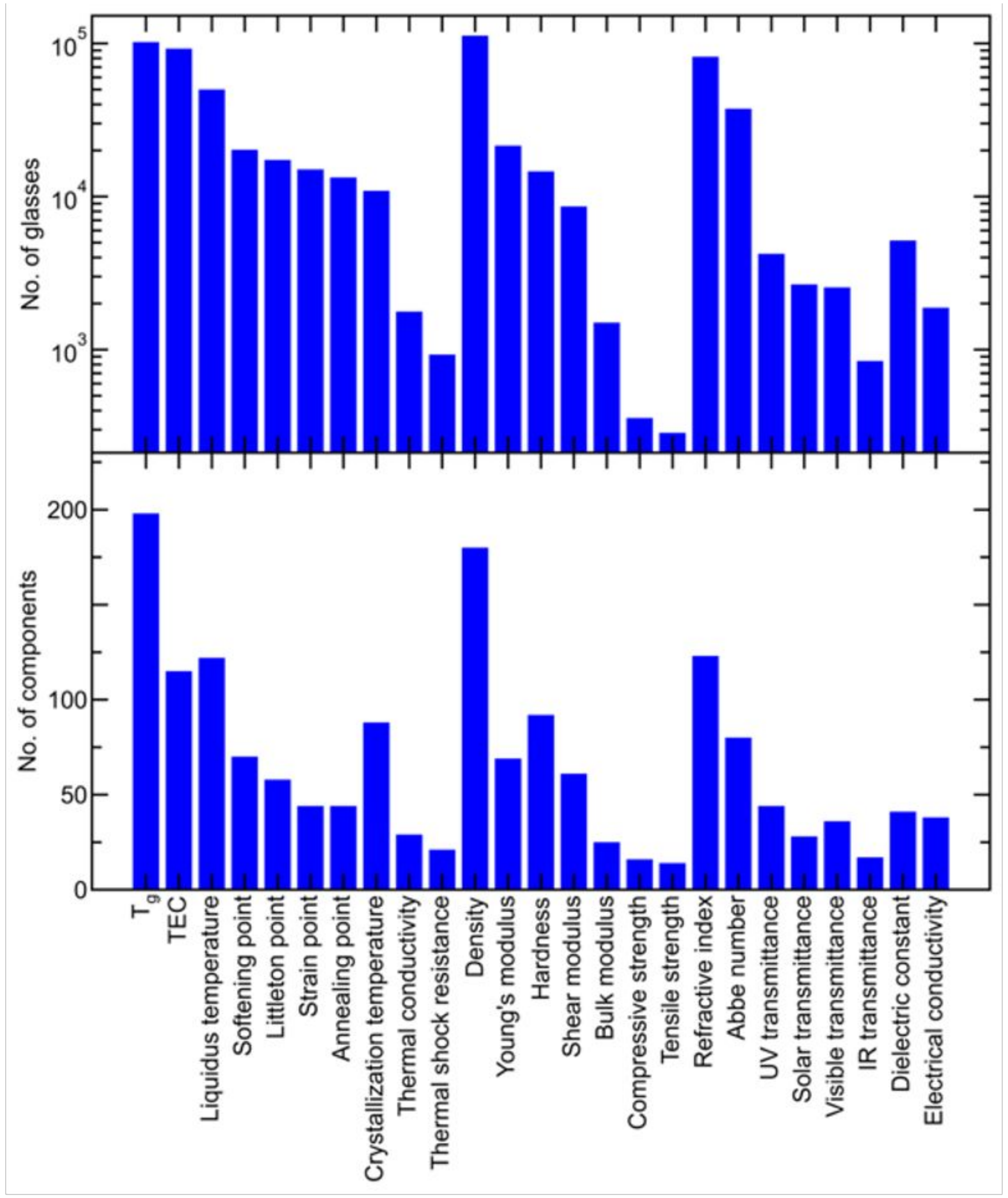
Gupta et al., NMAK, ACL, 2023; Hira et al., NMAK, AI4Mat, NeurIPS, 2024

Data-driven modeling in glasses



Dataset visualization

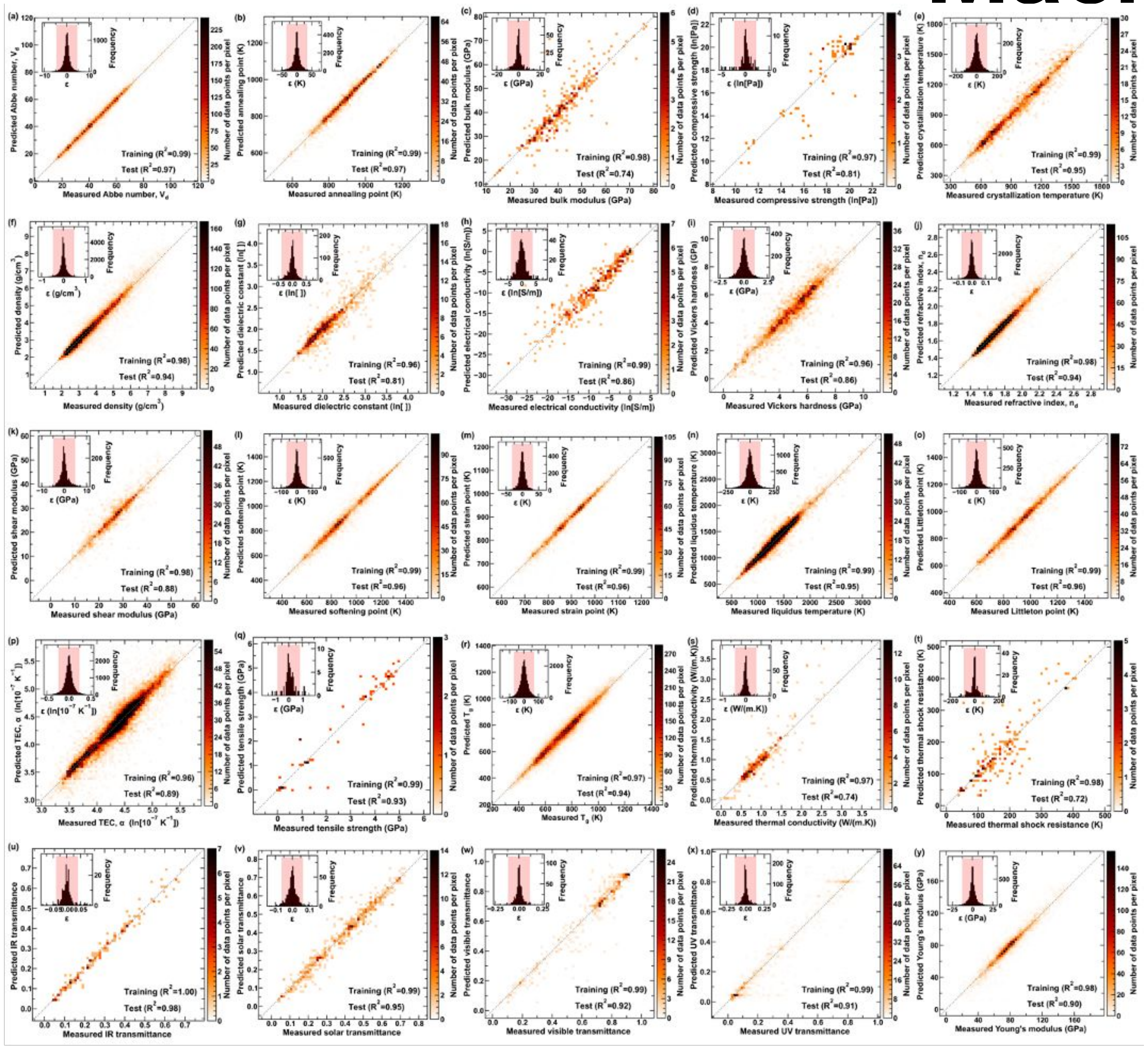


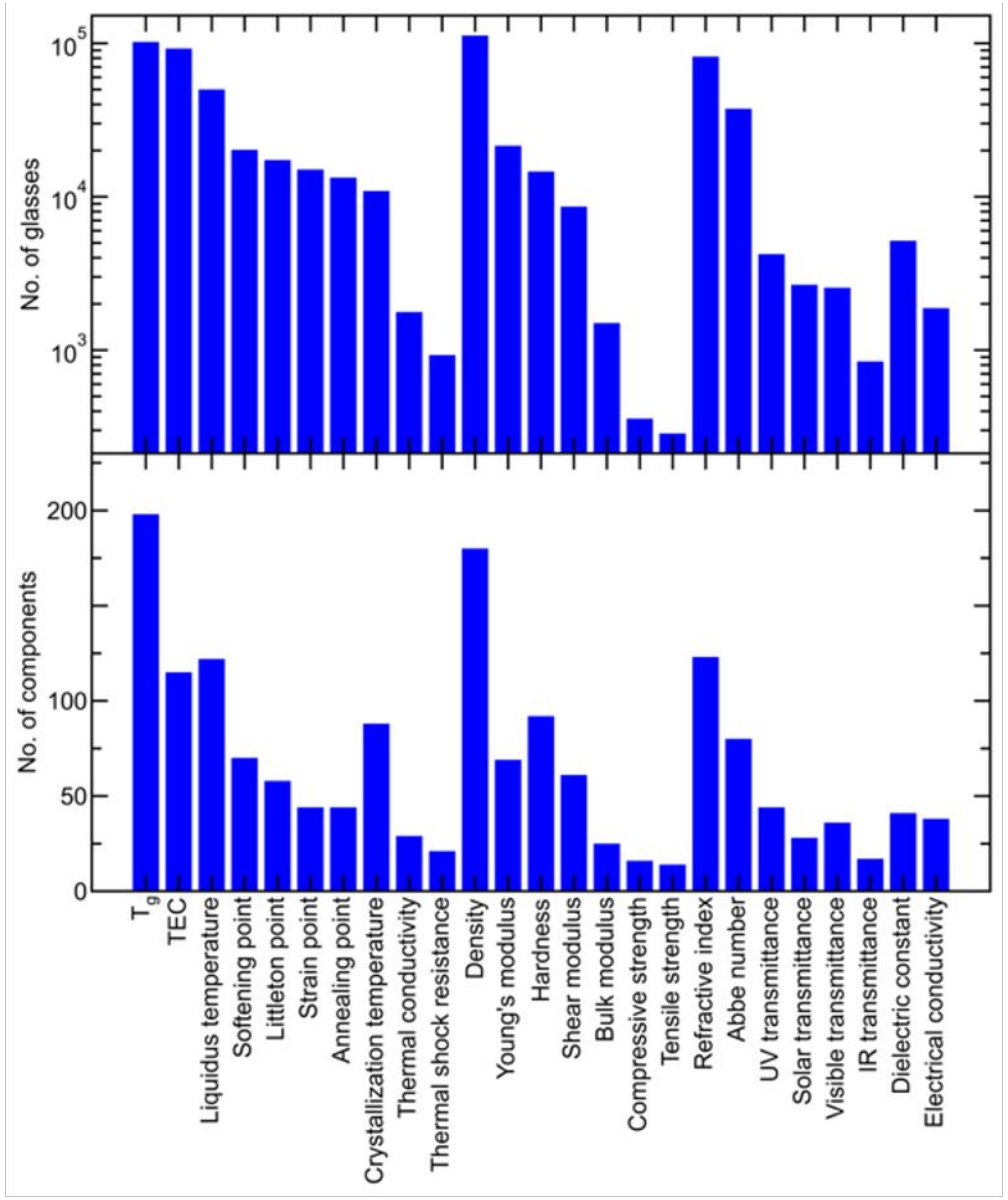


25 properties; 84 elements; 224 components; 450,000 glass compositions

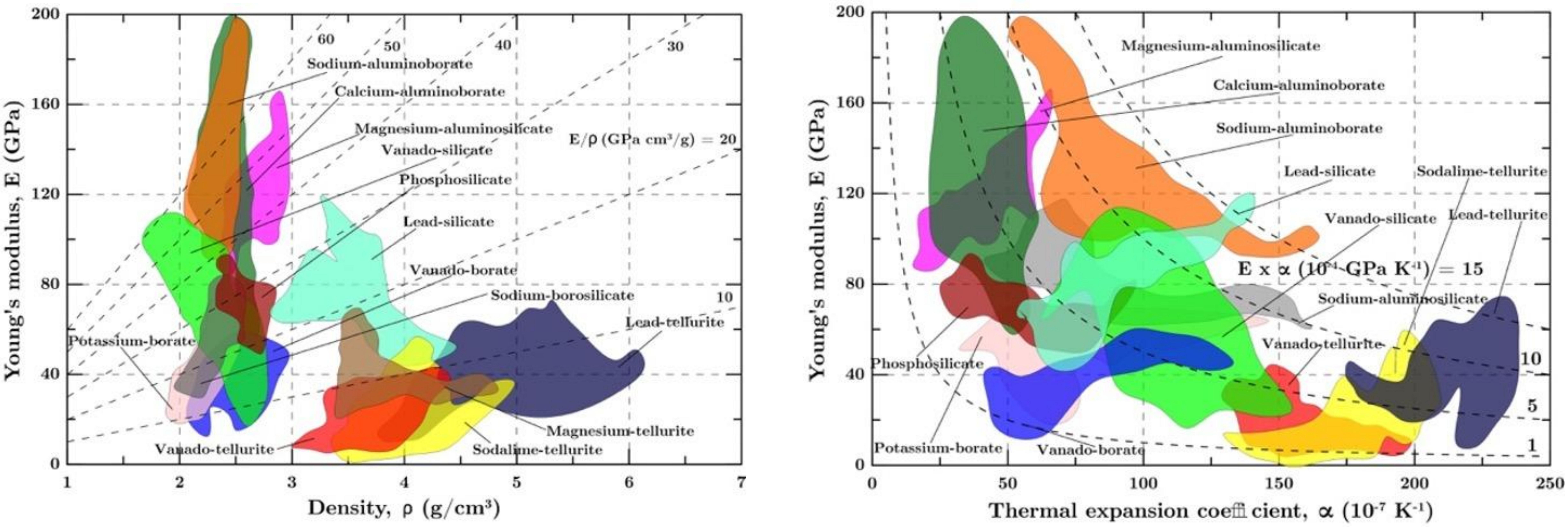
Bhattoo et al., NMAK, Materials Horizons, 2020; Bhattoo et al., NMAK, Acta Materialia, 2023

Machine learning models



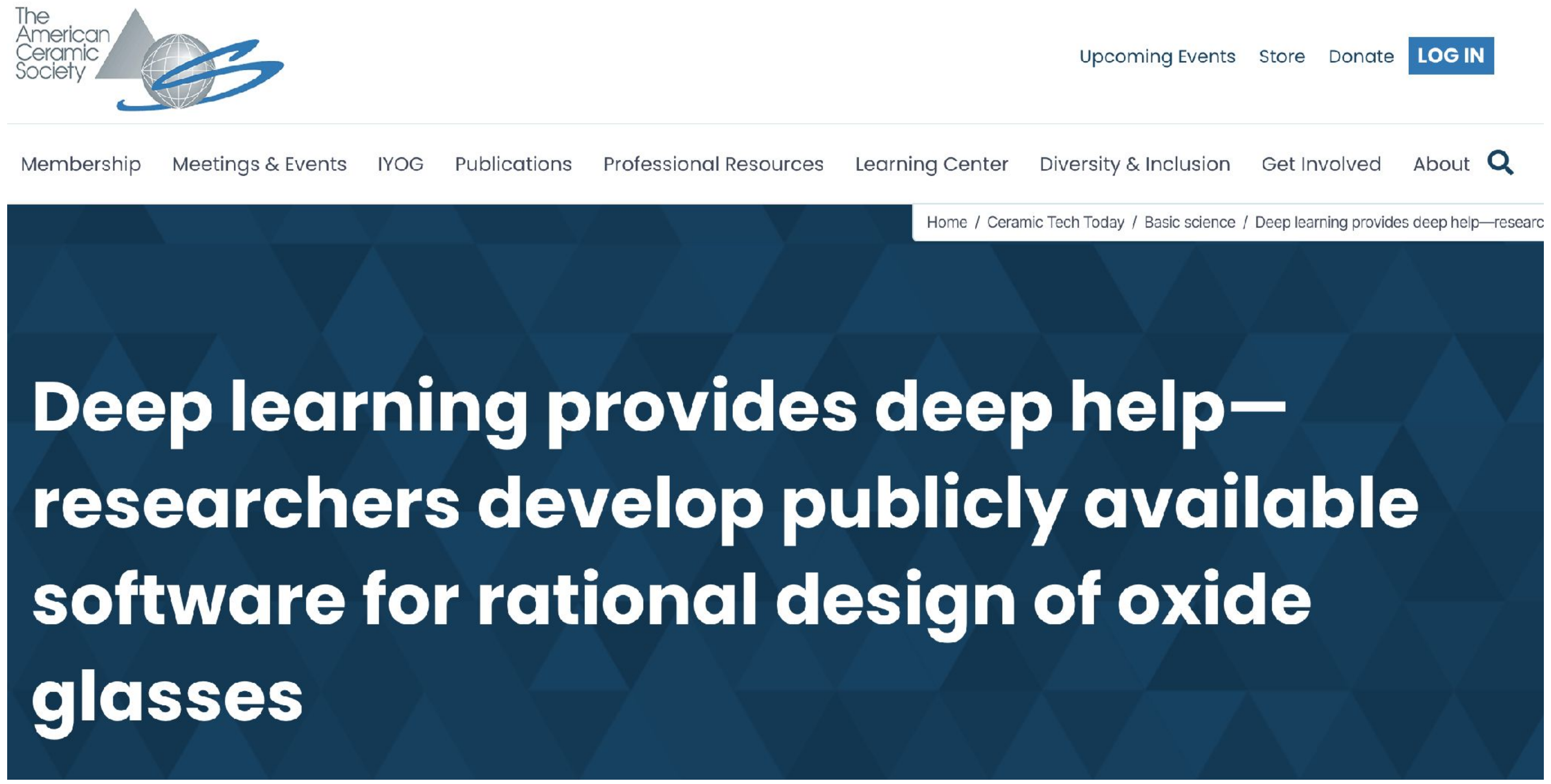


Material selection chart



Python for Glass Genomics (PyGGi)

http://pyggi.substantial.ai



- ISRO: Glasses for space application
- BRNS: Glasses for nuclear waste immobilization
- Sisecam: Glasses for commercial applications
- Battery electrolyte glasses

Case Studies

Constraints for nuclear waste glass

Composition constraints:

a) SiO_2+B_2O_3 ~ 60-70% (wt) is preferred with SiO_2 > 45% (wt) with B_2O_3> 10 wt%

b) Na_2O > 15% wt

c) Na_2O/B_2O3 > 1, preferably 1.25

d) ZnO ~ 2.5 – 10 wt% with a never exceed to 15% wt%

Property constraints:

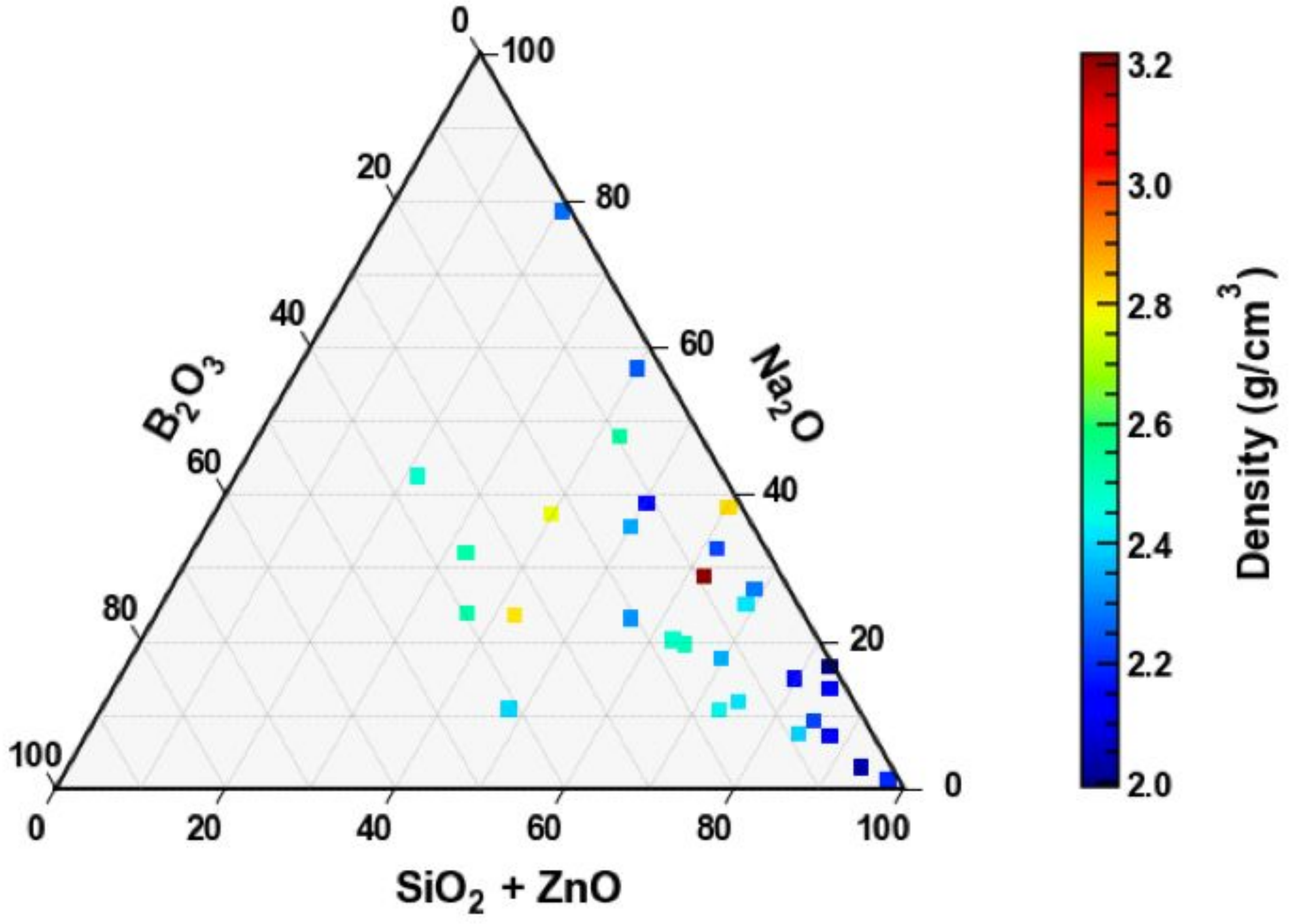
a) Tg value => 550 ^{0}C

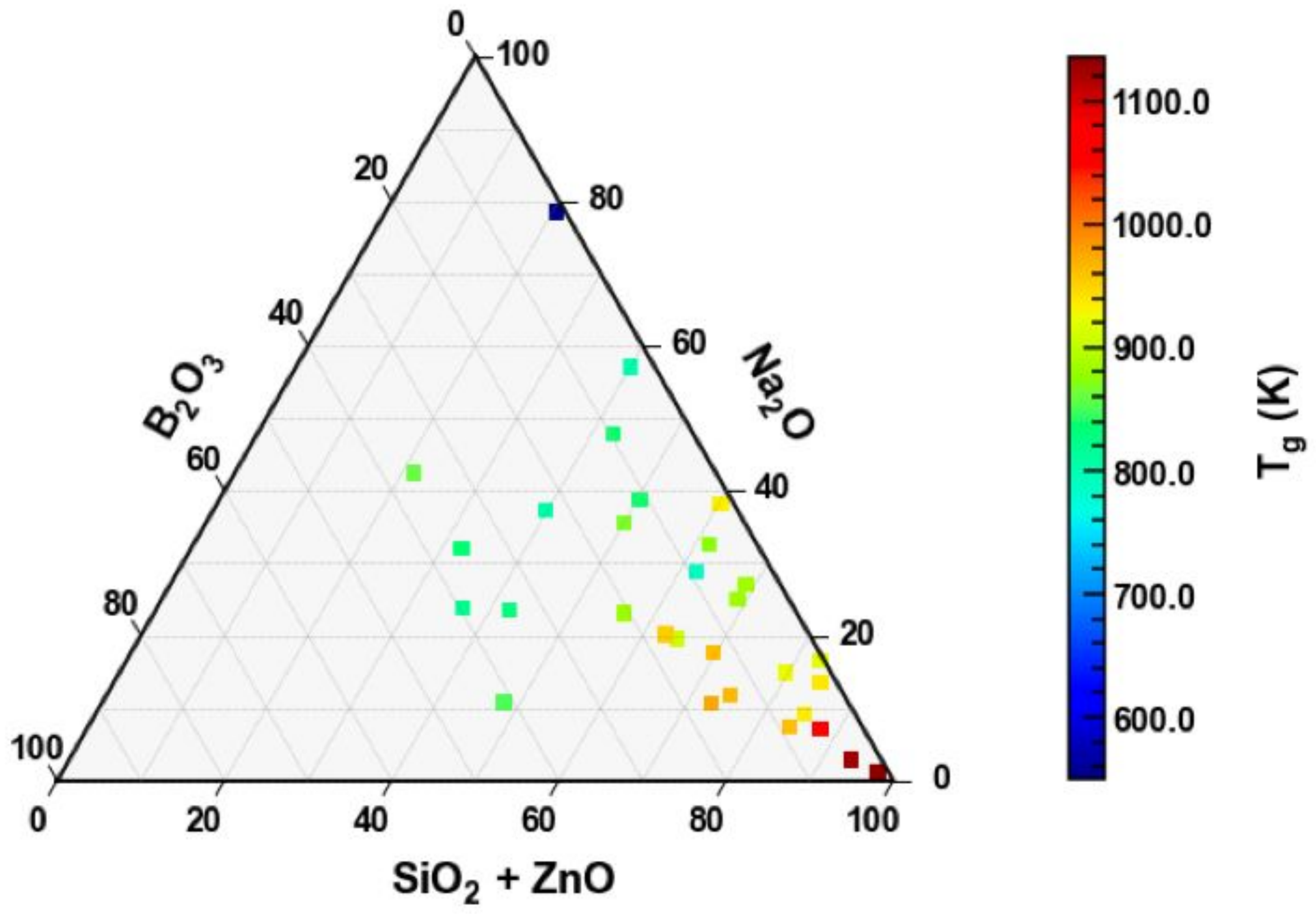
b) Density =2-3g/cm^3

c) Electrical conductivity = 50 S/cm

d) Viscosity > 50 poise at pouring temperature

e) Dissolution rate < 10^{-5} to 10^{-6} g/cm^2/day)





Optimized glass compositions

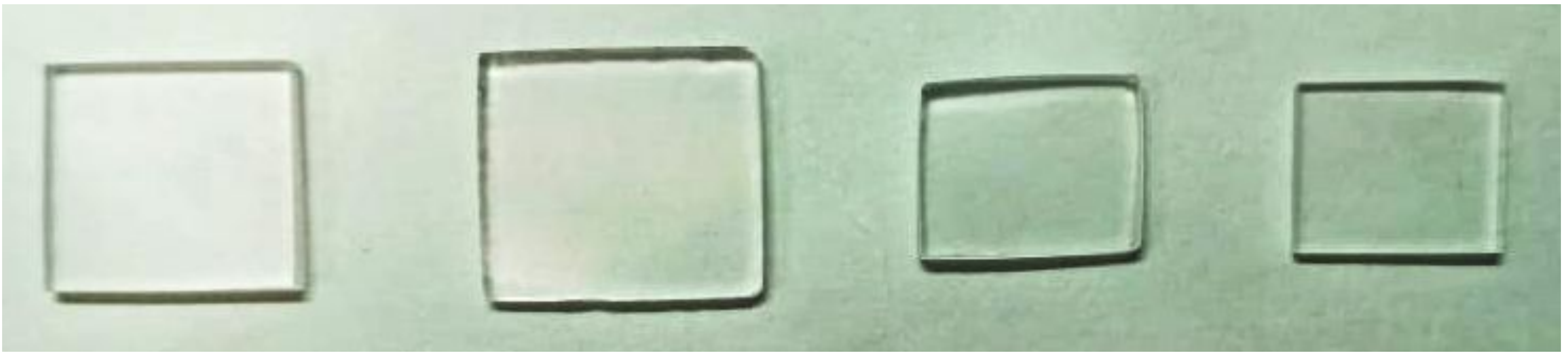
- Series of glasses obtained after compositional optimization using machine learned model

Na_2O (mol%)	SiO_2 (mol%)	B_2O_3 (mol%)	ZnO (mol%)	TEC (ln[10−7 K −1])	Thermal Conductivity (W/(m.K))	Density (g/cm3)	T_g (K)	Viscosity (poise)
21	52	18	9	101.90	0.77	2.62	808.87	2.6831
24	52	18	6	105.57	0.78	2.59	785.74	3.0581
27	52	18	3	114.34	0.77	2.51	776.94	3.5894
30	52	18	0	121.98	0.75	2.52	779.55	1.4328

Glass preparation

Sample Name	Na_2O	SiO_2	B_2O_3	ZnO
NBSZ-9	21	52	18	9
NBSZ-6	24	52	18	6
NBSZ-3	27	52	18	3
NBSZ-0	30	52	18	0

Temperature (℃)	Time (h)
0-300	3
300	4
300-800	5
800	4
800-1200	2
1200	1



Comparison between ML and experiments

Na_2O(mol%)	SiO_2 (mol %)	B_2O_3 (mol%)	ZnO (mol %)	TEC (ln[10−7 K −1])	Thermal Conductivity (W/(m. K))	Density predicted (g/cm^3)	Density measured (g/cm^3)	Tg (K)	T_g measured (K)
21	52	18	9	101.90	0.77	2.62	2.61	809	803
24	52	18	6	105.57	0.78	2.59	2.60	786	806
27	52	18	3	114.34	0.77	2.51	2.56	777	793
30	52	18	0	121.98	0.75	2.52	2.52	780	785

Constraints for pharmaceutical glass (Sisecam)

Target

Target	Value
Softening Point	1058 K
No. of Iterations	50

Property Constraints

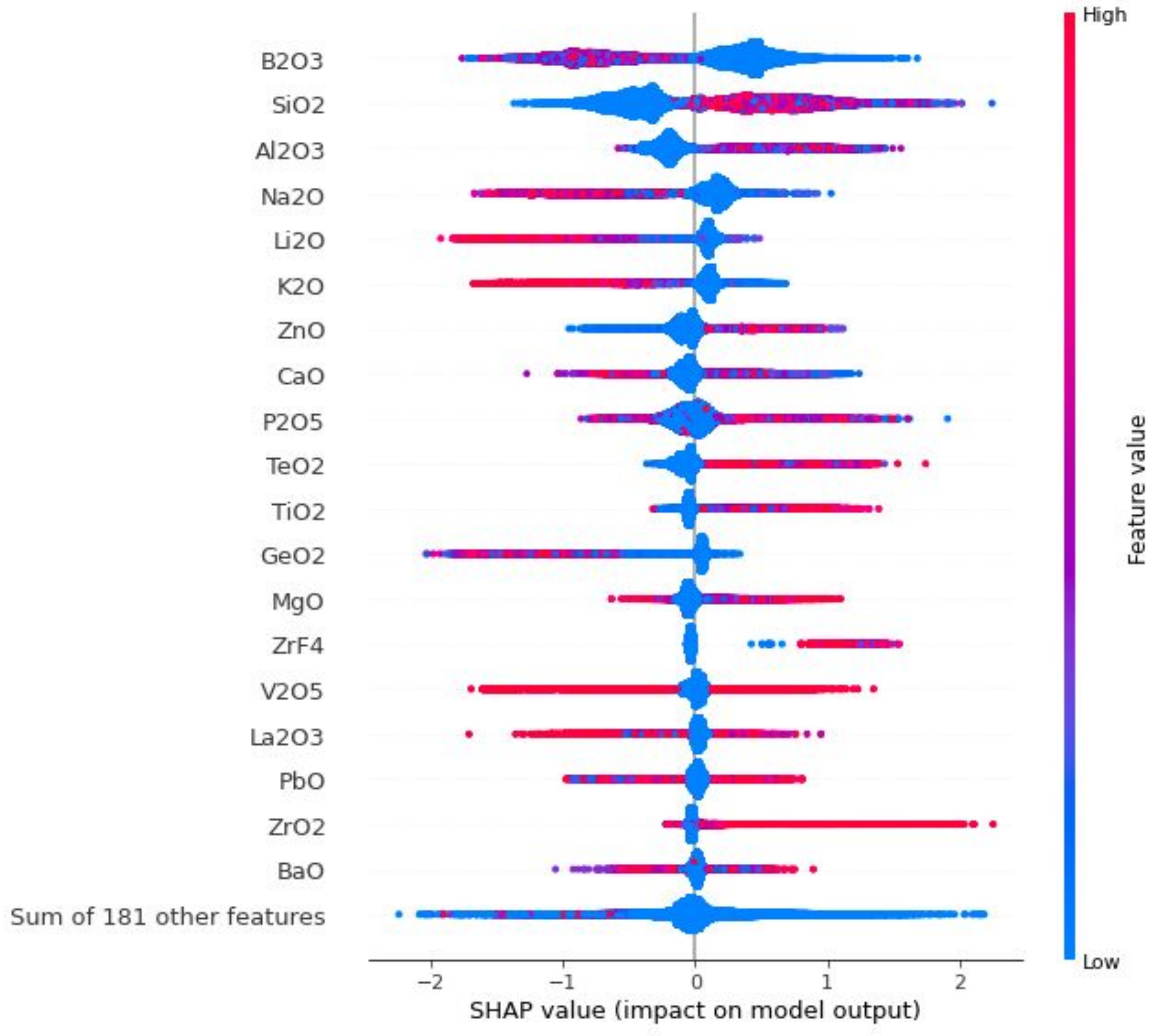
Property	Range
Glass Transition Temp.	833 – 843 K
Coeff. of Thermal Expansion	52 – 58 (x10 $^{-6}$)

Compositional constraints

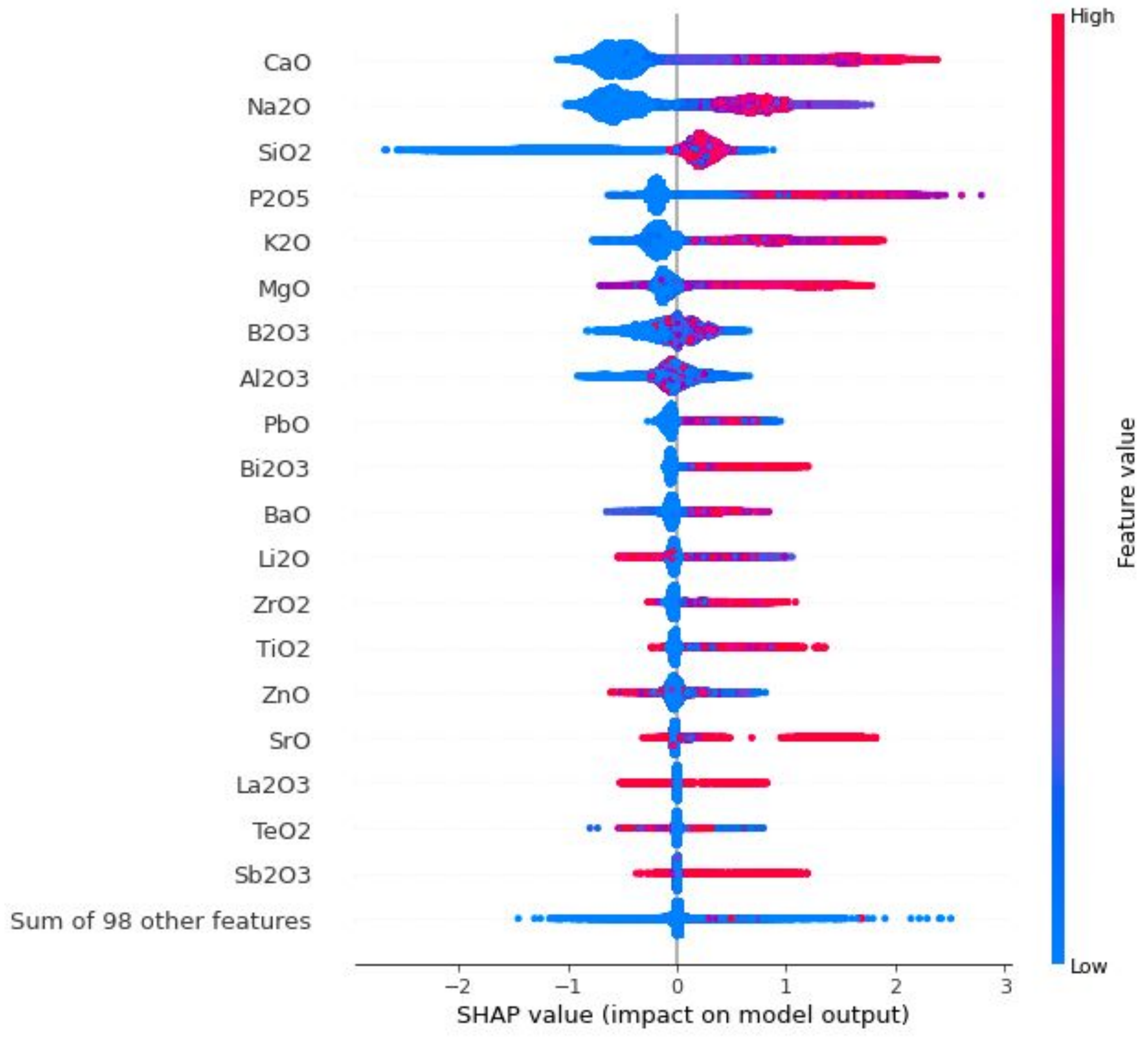
Component (wt%)	Range
SiO_2	67 - 77
B_2O_3	5 - 15
Al_2O_3	1 - 9
CaO	0 - 4
Li_2O	0 - 1
Na_2O	1 - 13

Constraints for pharmaceutical glass (Sisecam)

Interpretability



T_g



TEC

Towards Industrial Scale

Automation at Plant Level?

Cement manufacturing

- Cement manufacturing: an extremely complex process
- ~8% global CO_2 emissions
- Develop a digital twin for process optimization and quality control in collaboration 5 cement companies round the globe

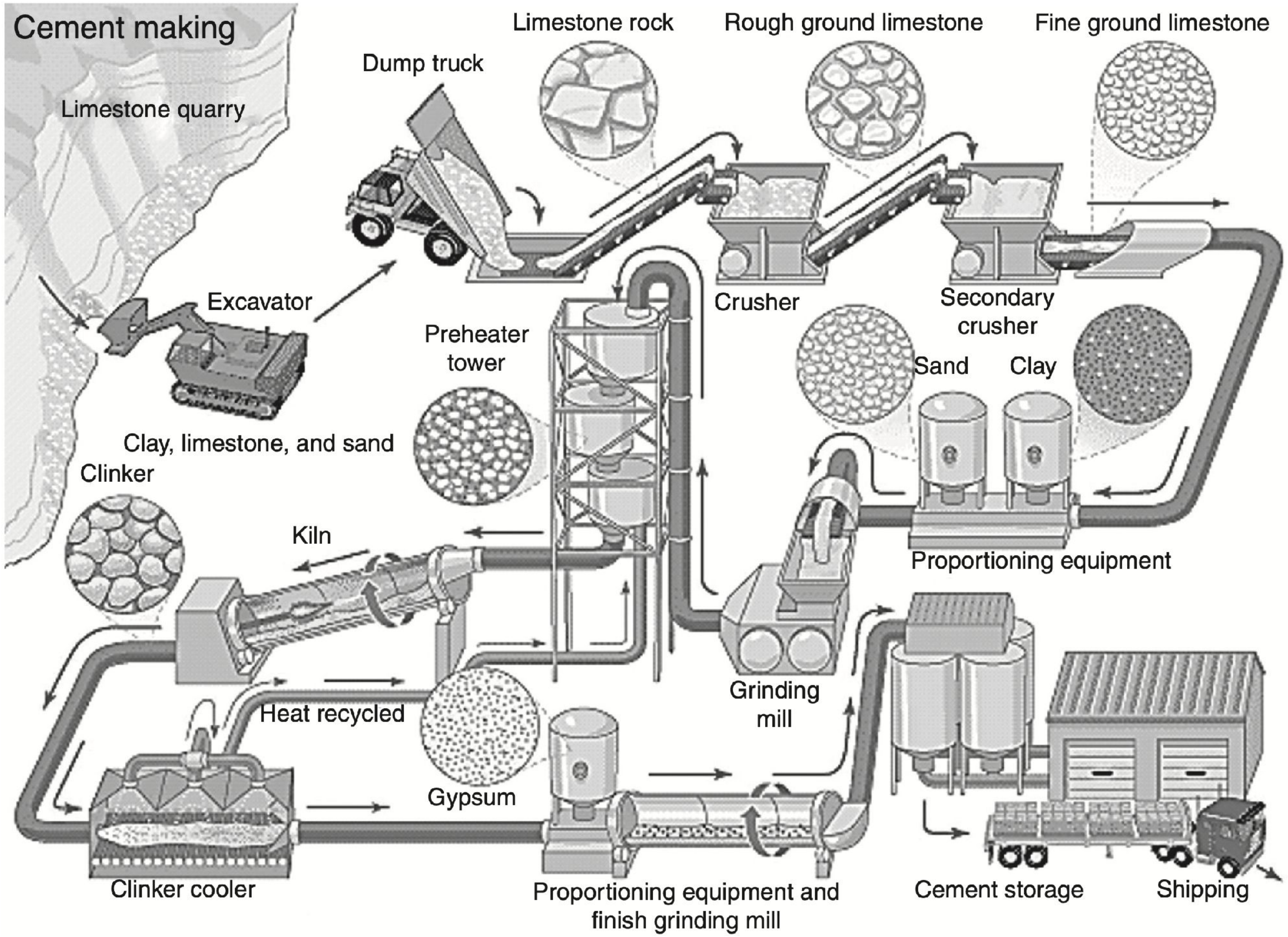
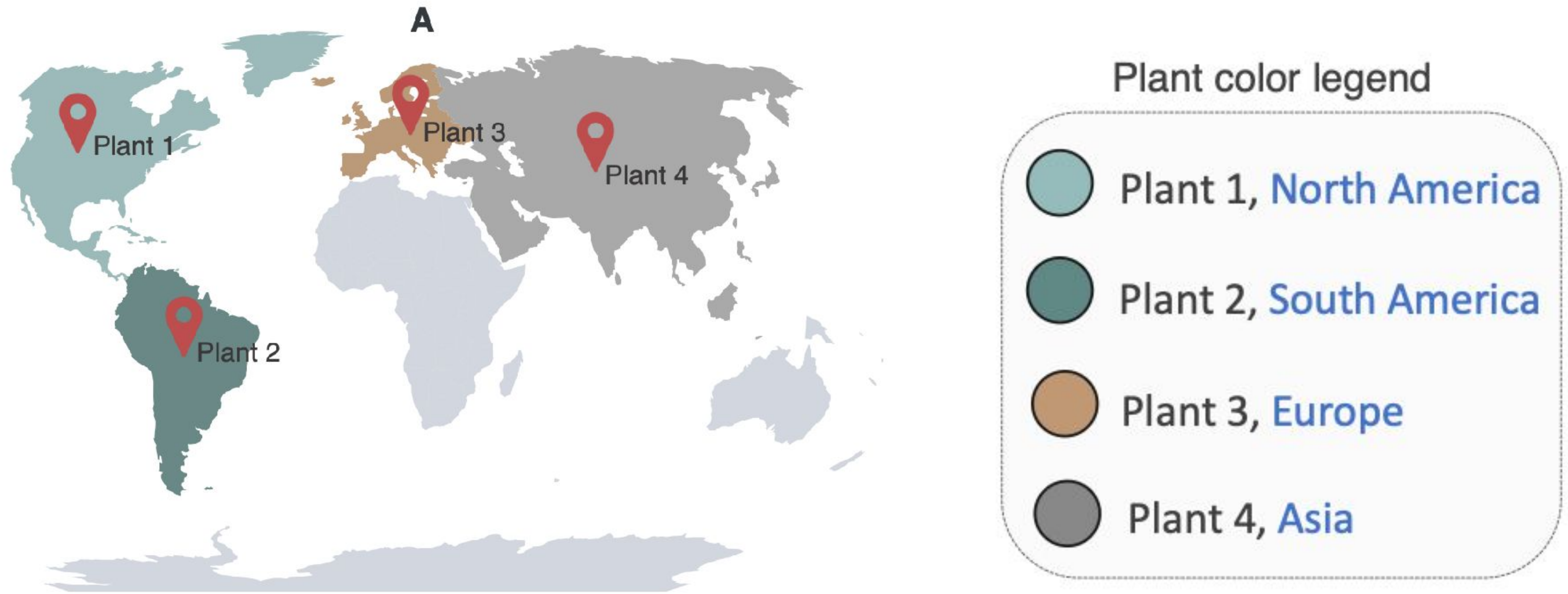


Image Source: Encyclopædia Britannica, Inc.

Data curation

Diversity : geography, fuel mix, configuration

Different levels of **data richness** :
Temporal granularity & data volume



Cement plant specifications				Data specifications							
								Size ‡			
ID	Location	Configuration	Fuel mix	Emissions measured (PPM)	Measurement location	Sampling frequency	Data Duration	Raw	After consistency check	After physical validation	After outlier removal
1	North America	5 stage PHT + ILC pre-calciner	Coal	NO_x CO CO_2	kiln inlet† (NO_x) stack end (CO) stack end (CO_2)	1 minute	01 Jan 20 - 31 Dec 21 (2 year)	1,052,567	894,036	277,603	277,079
2	South America	5 stage PHT + ILC pre-calciner	Petcoke, charcoal, waste wood chip, corn husk, rice husk, residual tires	NO_x	kiln inlet	2 hour	11 Jan 20 - 31 Dec 21 (2 year)	6,907	6,907	6,907	5,994
3	Europe	Reinforce suspension preheater (RSP) tower	Petcode, RDF	NO_x	kiln inlet	1 hour	30 Nov 21 - 22 Dec 22 (1 year)	5,784	2,621	2,621	1,620
4	Asia	6 stage PHT + ILC pre-calcienr	Petcoke, coal	CO	Stack end	1 hour	01 Feb 22 - 01 May 22 (3 months)	2,165	1,389	1,217	1,151

Emission prediction with historic inputs (EPH) models

Incorporating kiln-dynamics

$$y(t) = fEP[PP(t)]$$

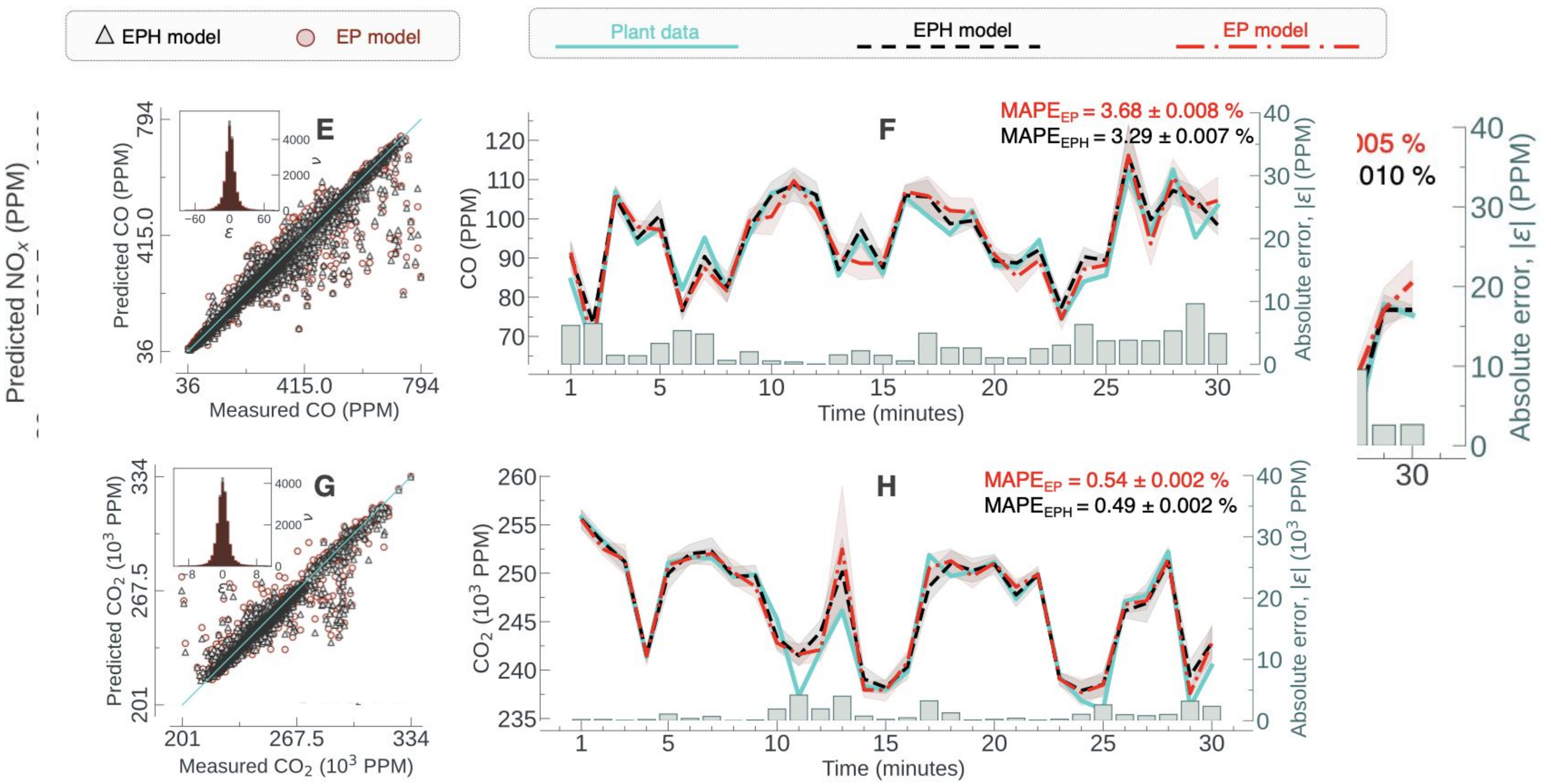
$$y(t) = fEPH[PP(t), PP(t-1), \ldots, PP(t-\tau)]$$

τ: *Process history*

Incorporate 20 min of process history (τ)

~3x reduction in NO_x error : 5.7% (EP) vs. 1.99% (EPH)

Dependence on prior operation



NO_x Control framework

DVs: Controllable process parameters

Constraints:

$\Delta|DV| \leq 5\%$

$\Delta RM_{flow\ chemistry} = 0$

$\Delta Fuel \leq 0$

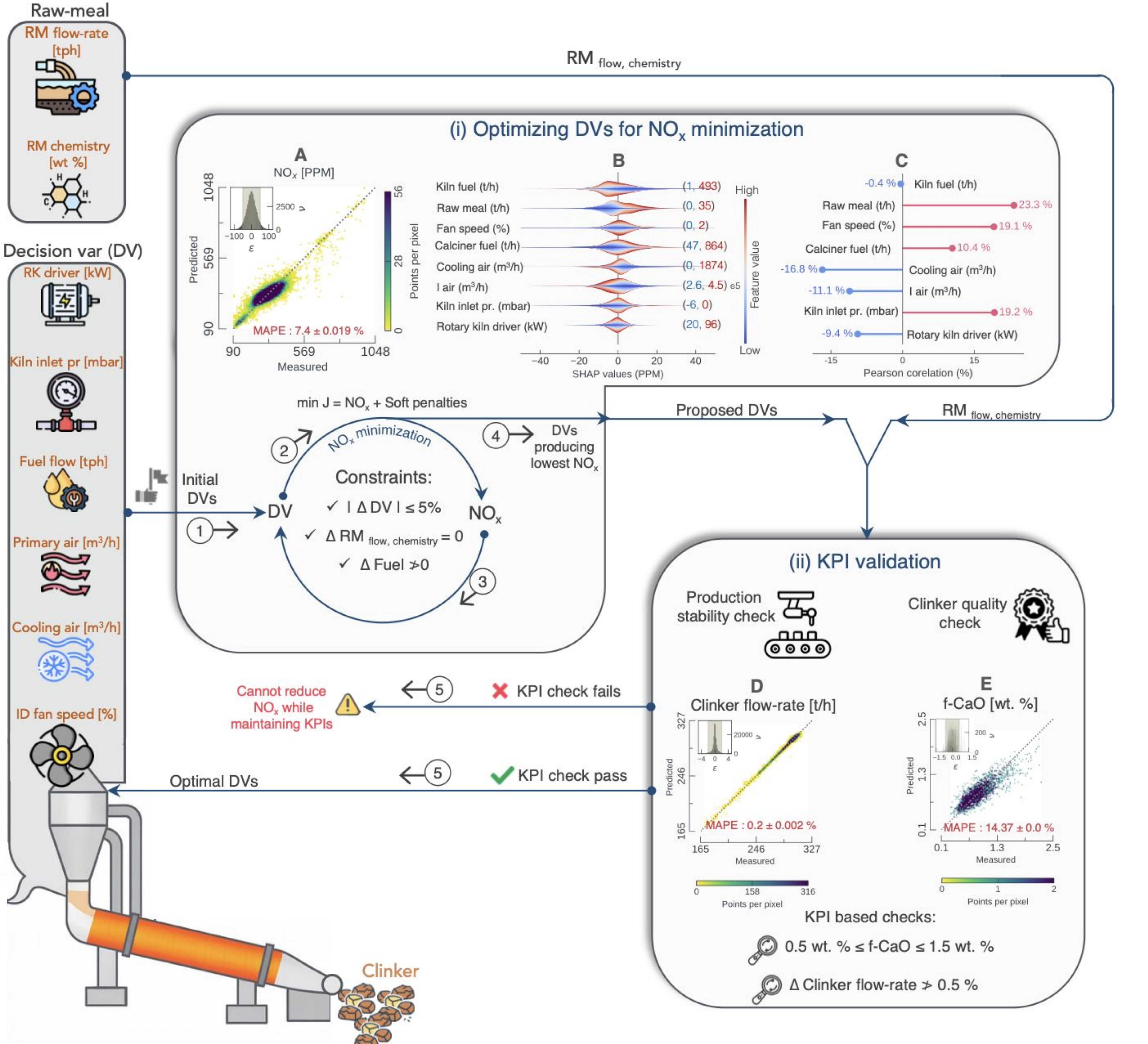
Objective function penalties:

Consistent with correlation & operational feasibility

KPI validation:

f-CaO ∈ [0.5 wt. % - 1.5 wt.%]

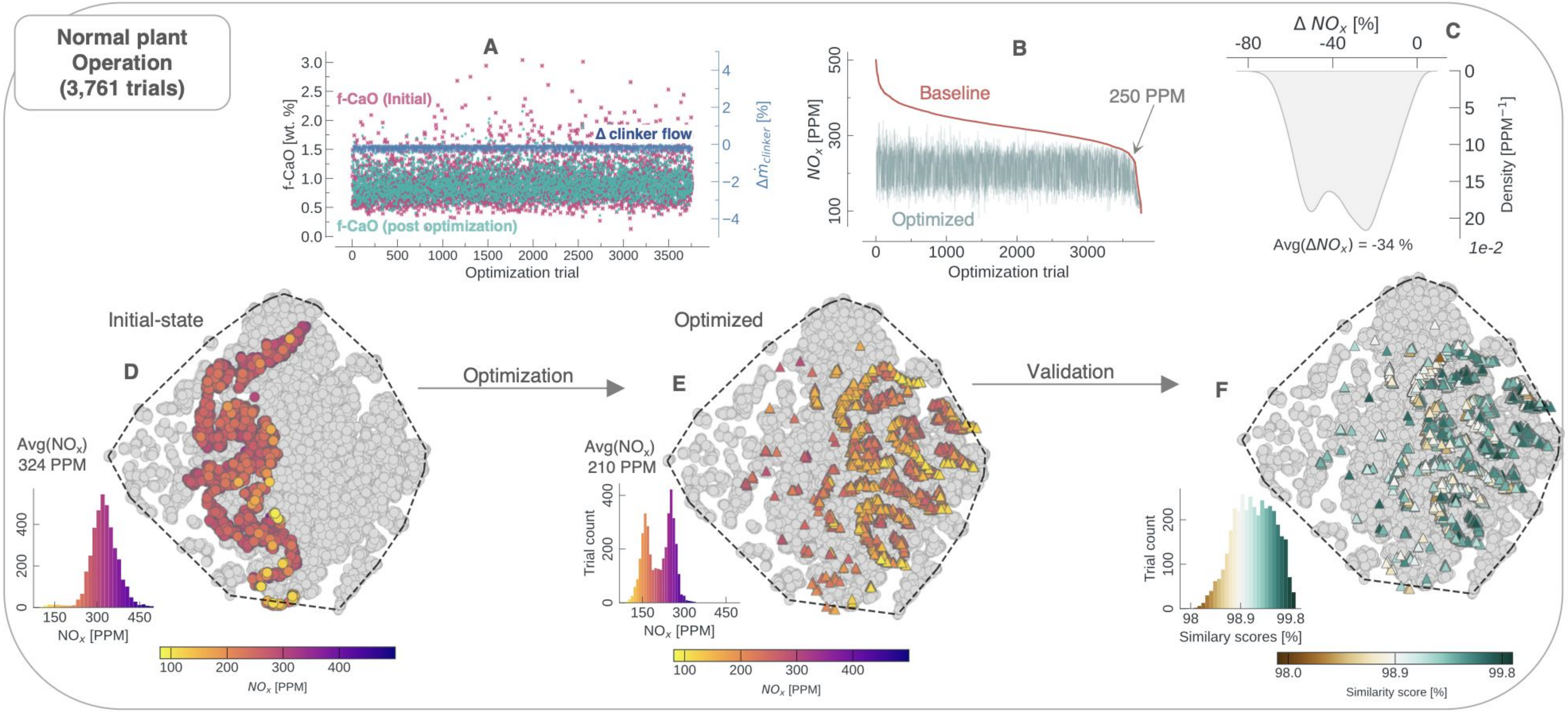
$\Delta\ Clinker\ flow \leq 0.5\%$



Controller performance

34% reduction

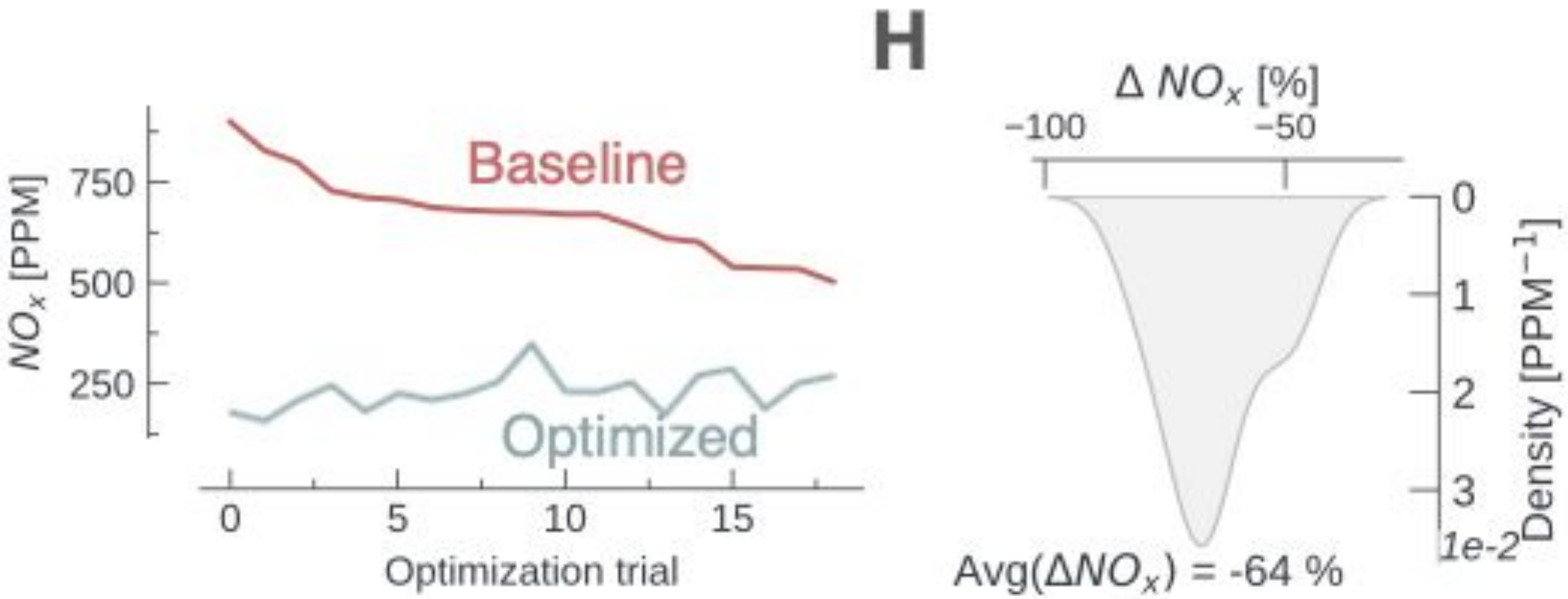
Scenario 1: Normal plant operation (NOx ≤ 500 ppm)



Controller performance

64% reduction

Scenario 2: Stress test (NOx > 500 ppm)



Techno-economic evaluation of the controller

2.3 Mt clinker/yr production

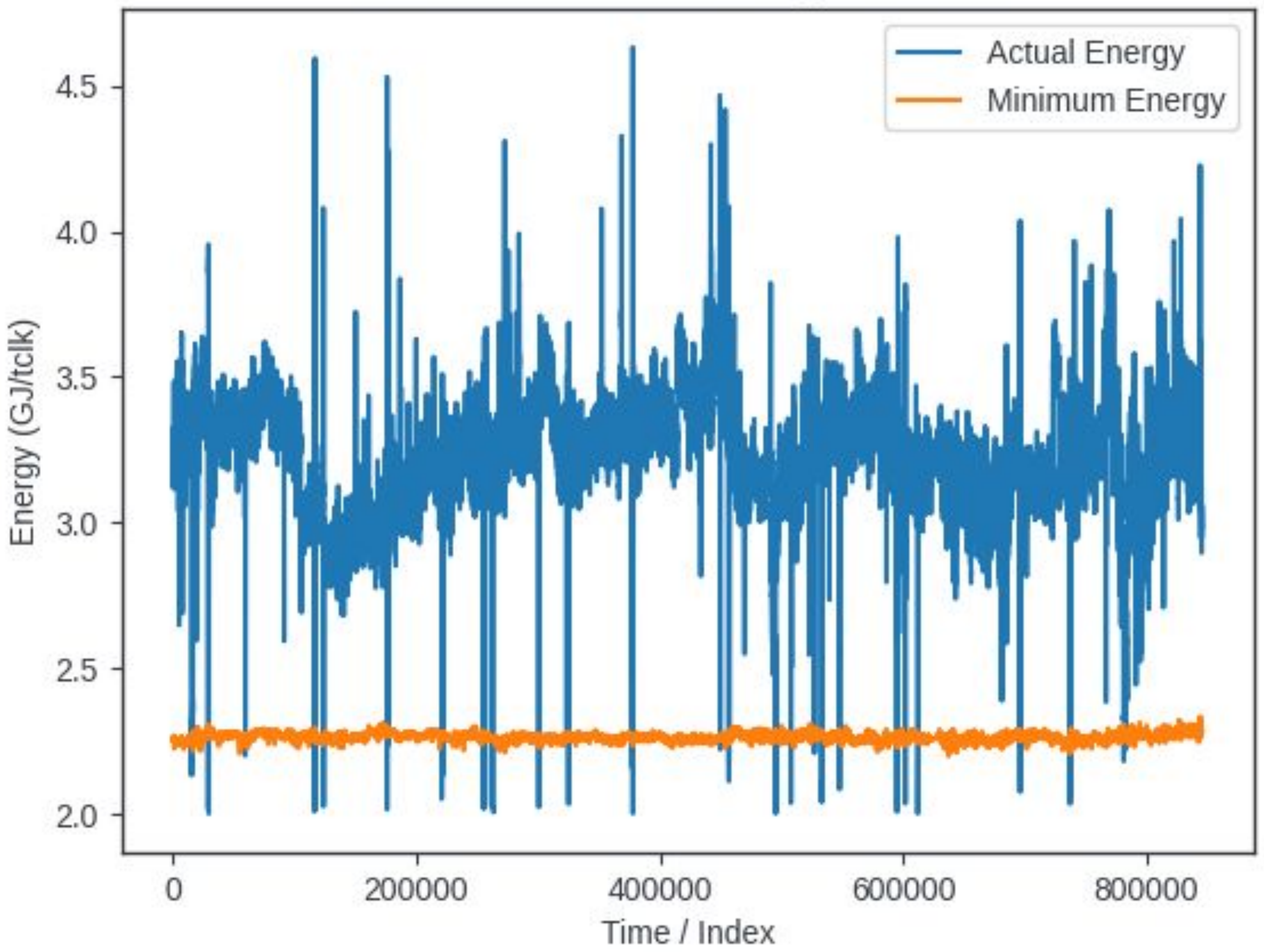
~290 t NO_x/yr controlled

~129 t NH_3/yr avoided

~58,000 USD/yr saved

[1] U.S. Environmental Protection Agency, Selective Noncatalytic Reduction (SNCR) for NOx Control: Technical and Cost Guidance, U.S. EPA, chapter 1 (SNCR process description, stoichiometry, NSR and reagent calculations) (2017).

Extension to fuel & CO_2 minimization



Mean actual = 3.2 GJ/ton clinker

Mean theoretical minimum = 2.3 GJ/ton clinker

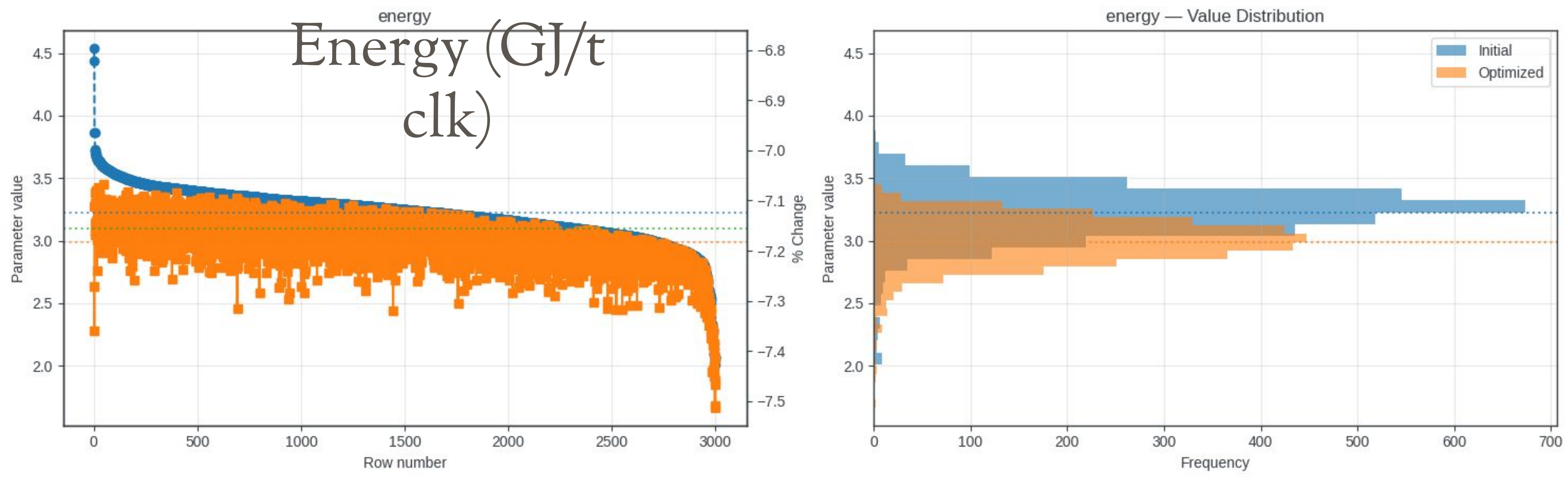
Initial values

Optimized values

Fuel reduction = 7.15%

Mean Initial: 3.226 | Mean Optimized: 2.992 | Mean % Change: -7.15%

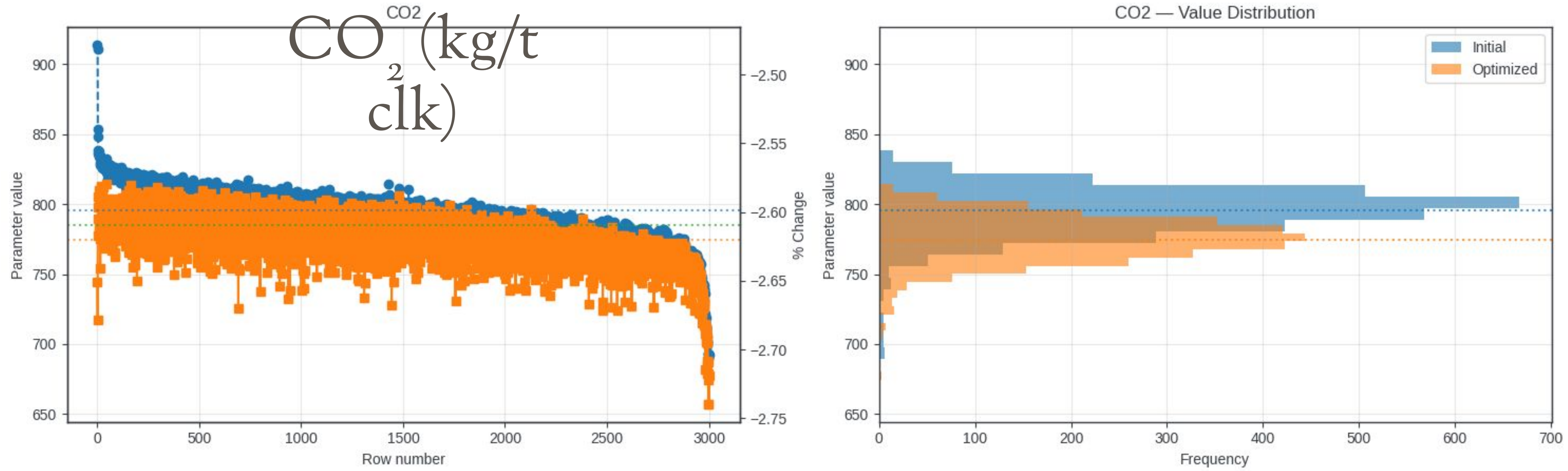
Energy (GJ/t clk)



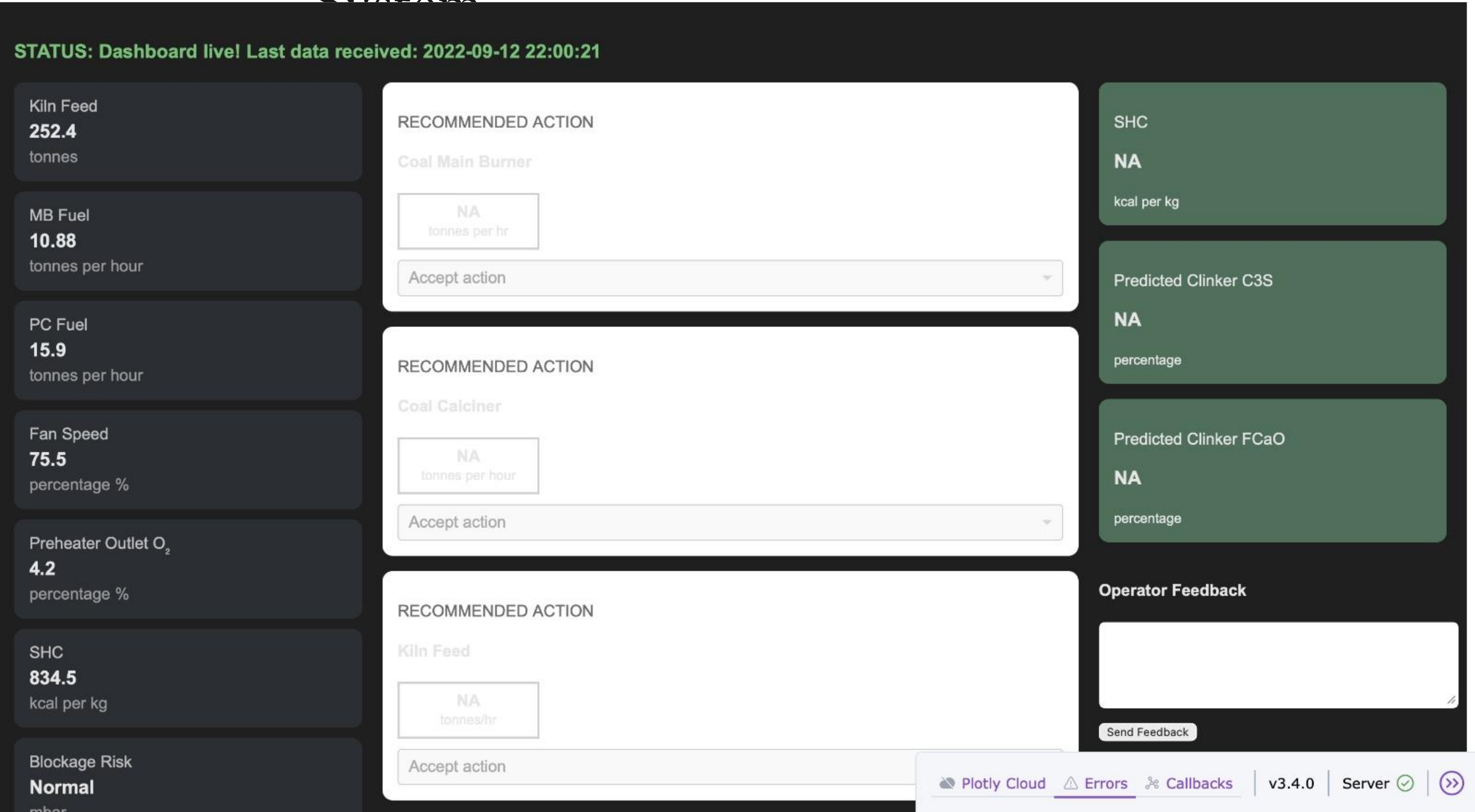
Corresponding CO_2 reduction = 2.61%

Mean Initial: 795.277 | Mean Optimized: 774.413 | Mean % Change: -2.61%

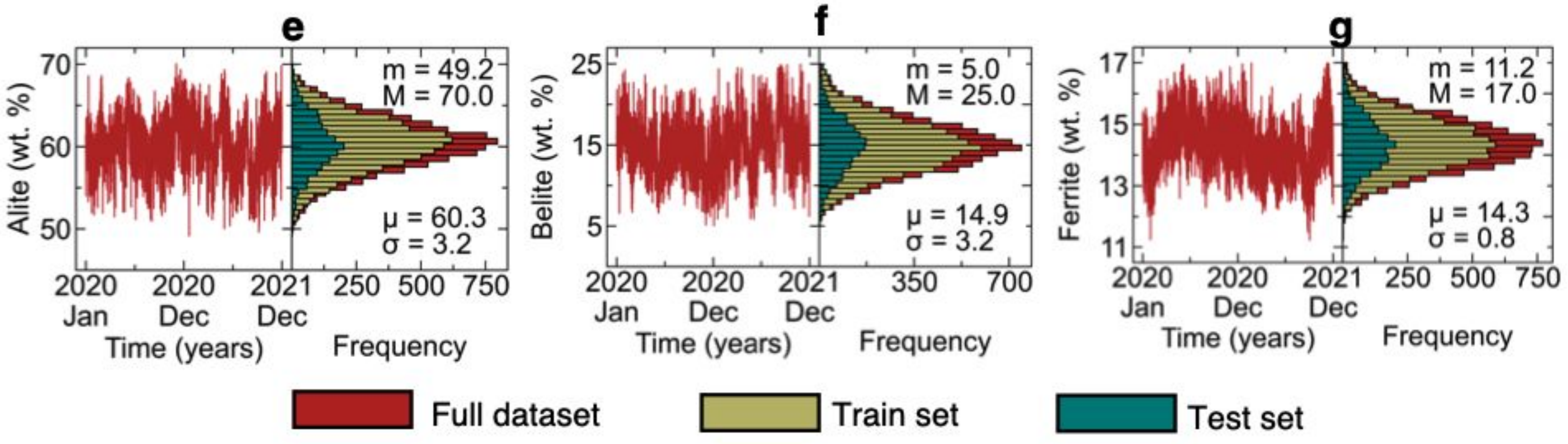
CO_2 (kg/t clk)

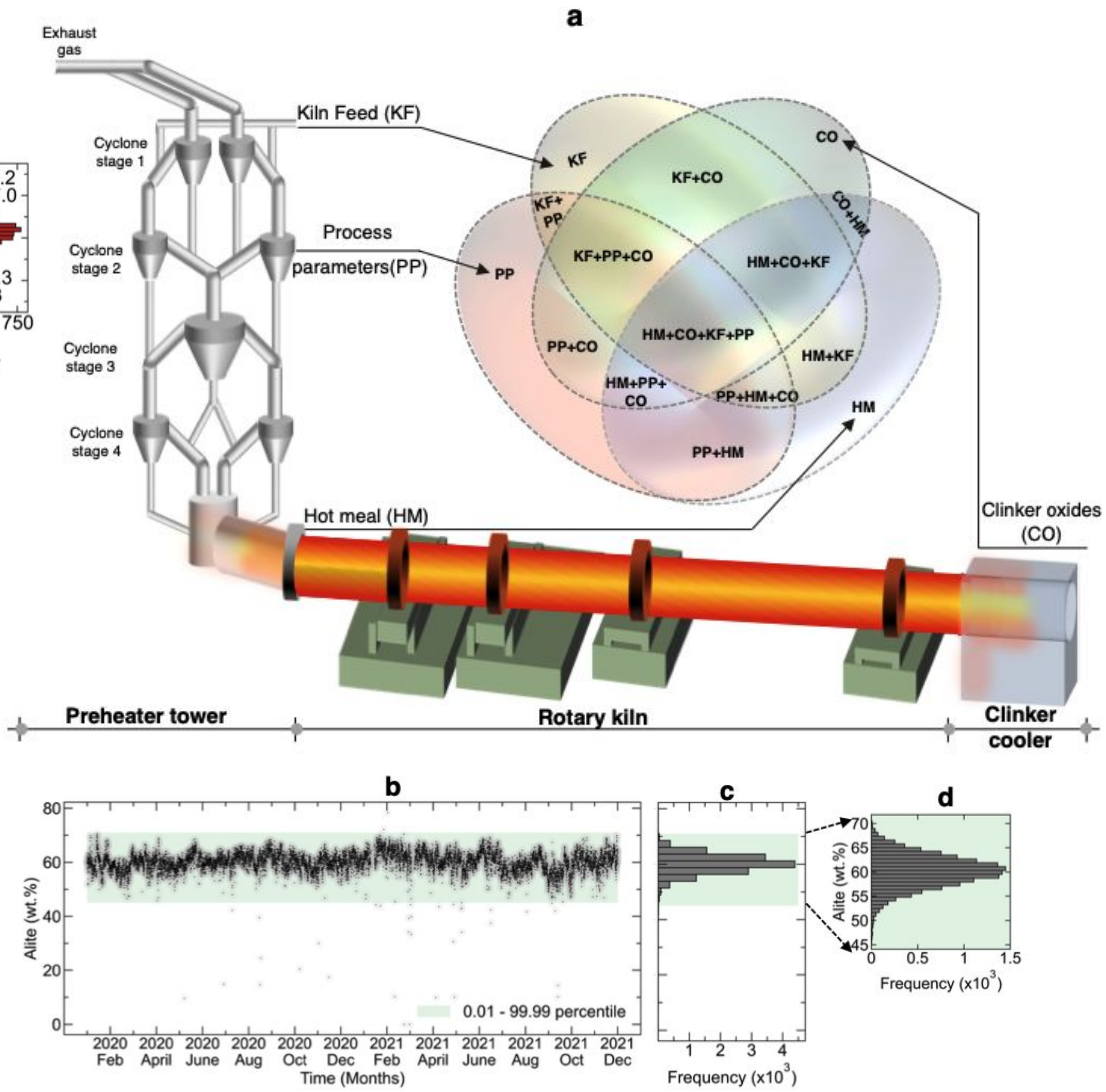


Agentic Decision Support System



Model features



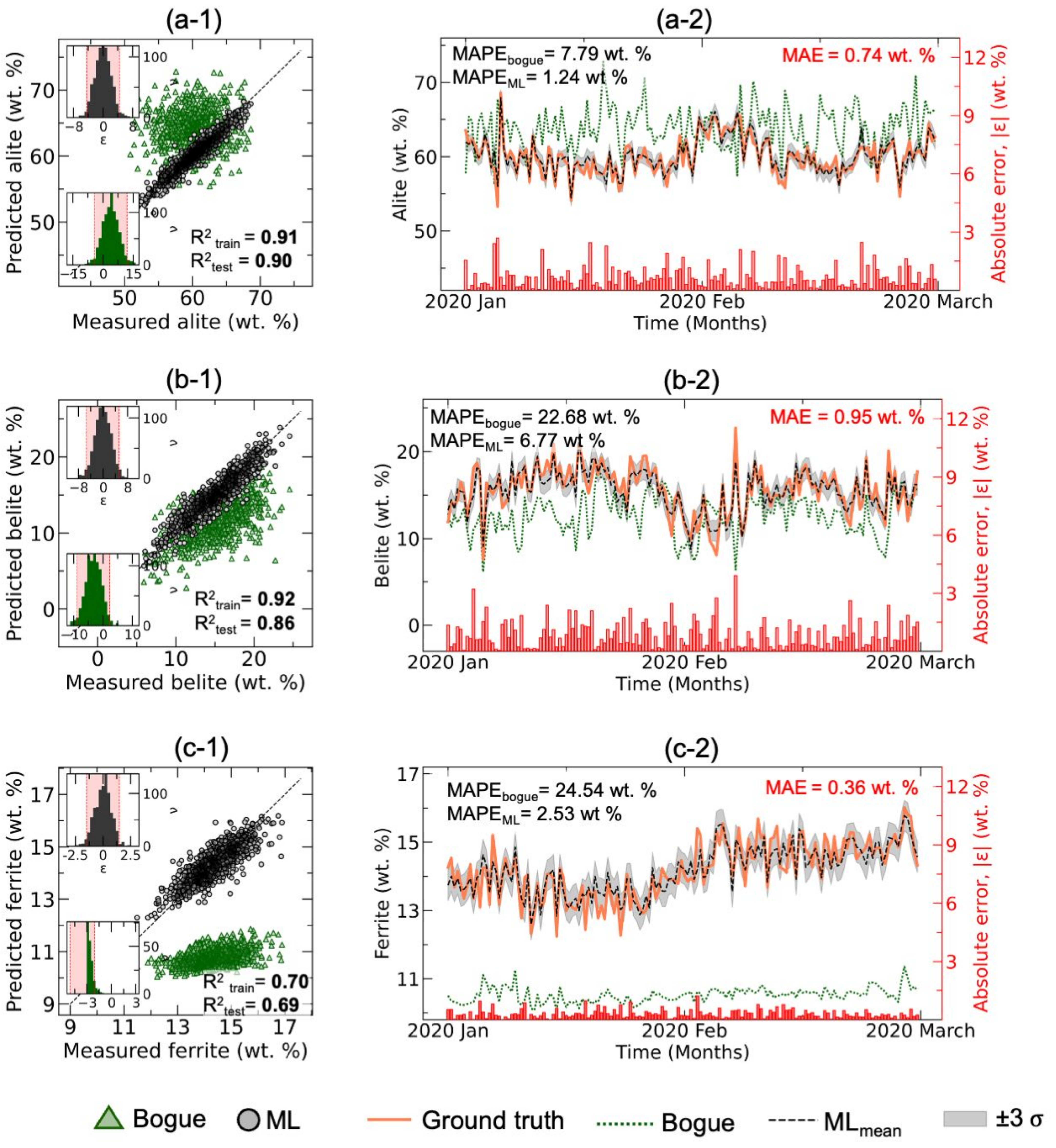


- Input features include raw materials, fuel, process parameters

- Goal: Clinker mineralogy

- Major challenge: Data cleaning and alignment

Model performance



- Accurately forecast clinker compositions
- Allows direct control of the plant for optimization
- Performs better than the models employed in the plant

Way forward: Proposal

Industry Academia joint Center of Excellence/Consortia on Glass

- Goal: Towards Sustainable Glass Manufacturing and leadership in Glass Industry
- Problem statements of industrial relevance proposed by Industry
- Mentorship from both academia and industry
- What we have: Strong industry, world-class research, increasing demand (unlike several other parts of the world)


Mausam


K. Jablonka


Indrajeet Mandal

Thank you!


Sajid Mannan


Vinay Kumar

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High Performance Computing at IITD

Supercomputer @ IITD : The Central Hybrid Supercomputing Cluster at Indian Institute of Technology Delhi

Alexander von HUMBOLDT STIFTUNG

Google DeepMind

Undergraduate and doctoral researchers at M3RG, IIT Delhi

Thank you!

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