Understanding Where AI Adds Value in R&D:

Accelerating Materials Discovery

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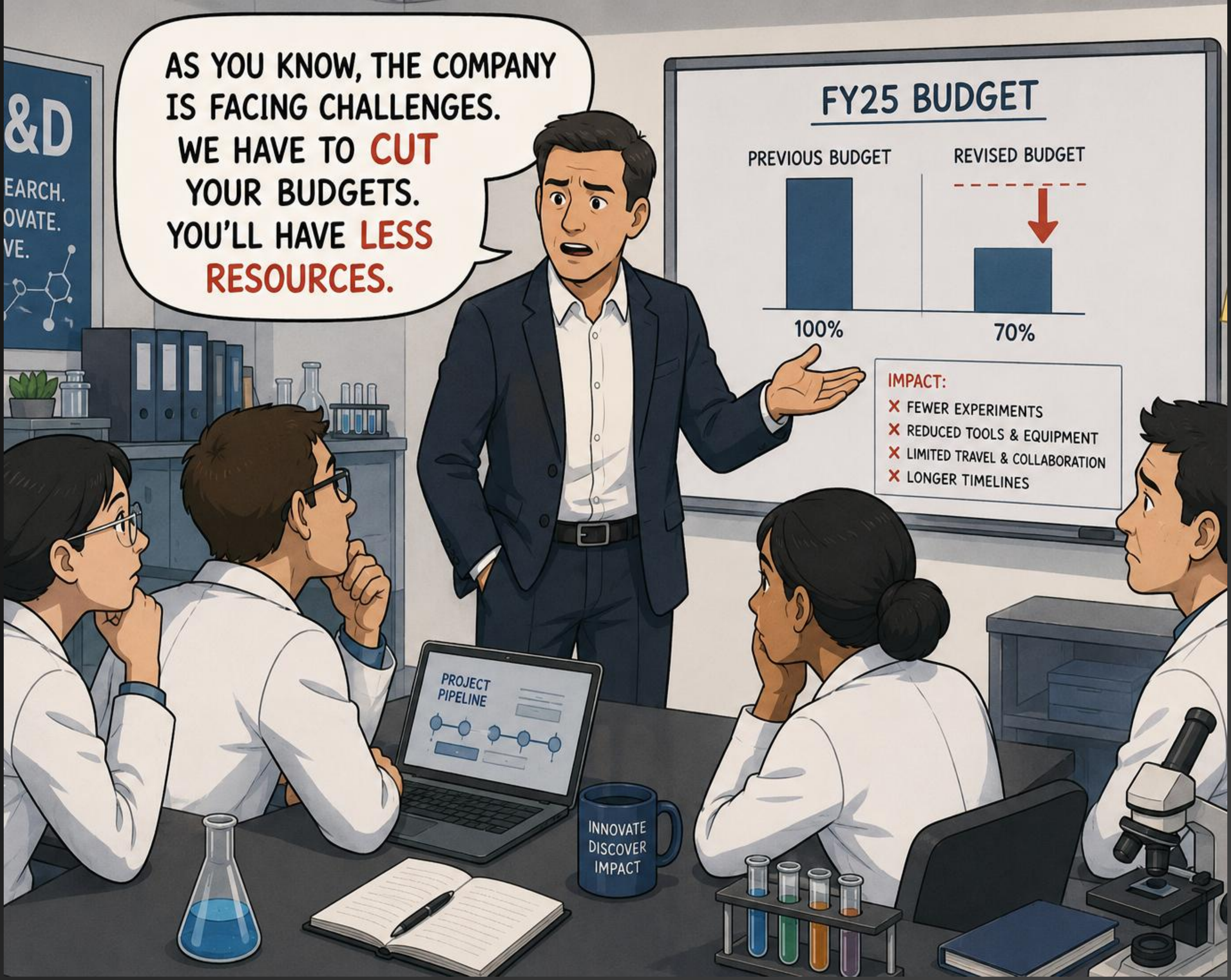
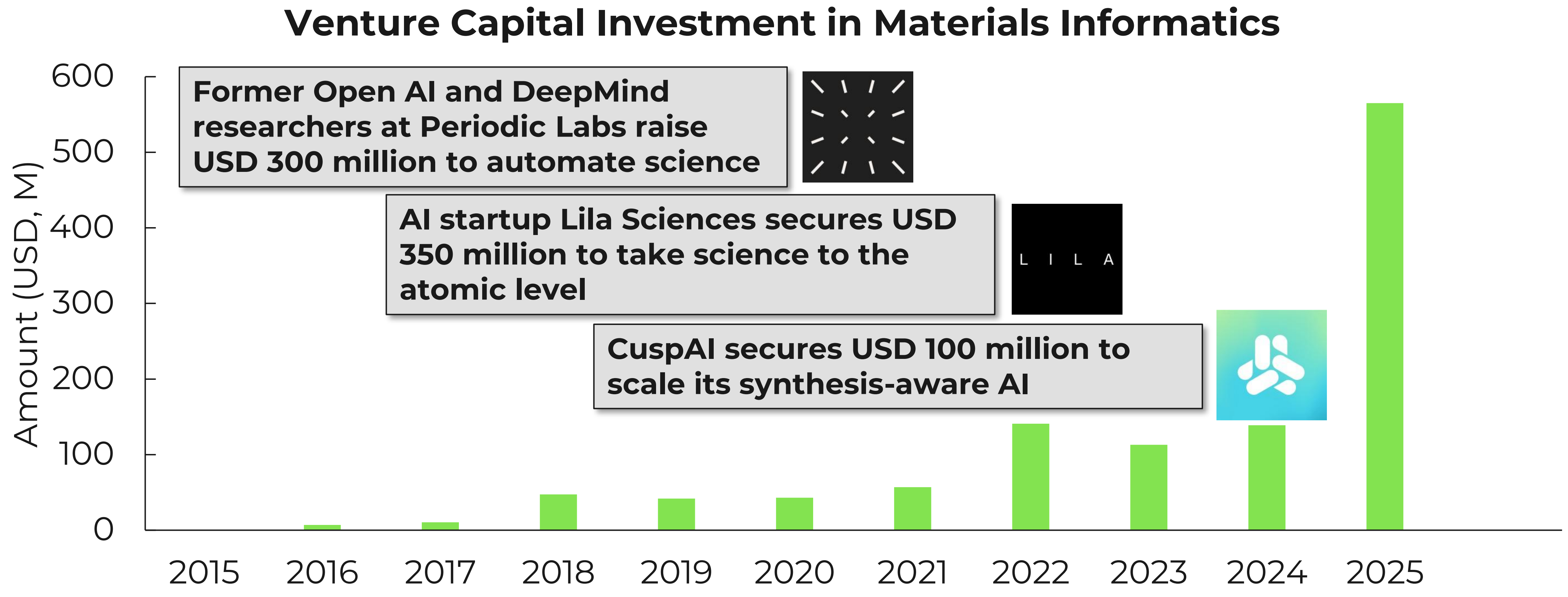
WE NEED NEW MATERIALS—
FASTER!
I NEED BREAKTHROUGHS,
NOT TIMELINES.
MOVE FASTER!
R&D
INNOVATE.
DISCOVER.
TRANSFORM.
BETTER
MATERIALS
BETTER
FUTURE
OUR GOAL:
INVENT NEW MATERIALS
FASTER
PERFORMANCE
SUSTAINABILITY
SCALABILITY
IMPACT
NEW MATERIALS
IDEAS
SCIENCE
DRIVES
PROGRESS
MATERIALS SCIENCE
POLYMER INNOVATION
ADVANCED ALLOYS
NANOMATERIALS



Source: ChatGPT

Let me ChatGPT this....

AI companies are raising millions




DREAMING NEW MATERIALS
IMAGINE > DESIGN > GENERATE > DISCOVER
CRYSTAL LATTICES
MOLECULAR STRUCTURES
POLYMER CHAINS
METALLIC MICROSTRUCTURES
BATTERY MATERIALS
POROUS FRAMEWORKS

AI can dream, but can it realize those dreams?

Agenda

01 | Evaluating AI’s value across the materials development workflow

02 | Diving deep into specific materials examples

03 | Looking ahead for AI-enabled materials R&D

Basic materials development workflow

01 **Design**

02 **Synthesis**

03 **Processing**

04 **Characterization**

05 **Testing**

06 **Scale-up**

Each step has multiple sub-steps to consider

01 Design
- Molecule selection
- Structure / system design

02 Synthesis
- Materials preparation
- Process control
- Yield optimization

03 Processing
- Component selection
- Mixing/ structuring
- Process tuning

04 Characterization
- Structural / molecular
- Morphology / surface
- Property measurement

05 Testing
- Performance testing
- Stability / durability
- Specialized validation

06 Scale-up
- Process scale-up
- Process optimization
- Manufacturing integration

AI applications span every step

01 Design	02 Synthesis	03 Processing	04 Characterization	05 Testing	06 Scale-up

- LLMs for review
- Accelerated DFT
- Generative molecular design
- Automated synthesis and high throughout experimentation
- Design of experiments optimization
- ML models for characterization and testing
- Process digital twins
- R&D management platforms

So, there are many ways AI could plausibly help

01 Design | **02 Synthesis** | **03 Processing** | **04 Characterization** | **05 Testing** | **06 Scale-up**

LLMs for review

Accelerated DFT

Faster iterations, improved accuracy, novel molecules

Automated synthesis and high throughout experimentation

Design of experiments optimization

Reduction of up to 50%–60% in number of experiments, reducing in cost, reduce material waste, accelerated time to market, safe screening and optimization

Automated characterization and testing

R&D management platforms

Process digital twins

Faster multi-objective yield optimization

A 3-step process for prioritizing AI opportunities

1.
Evaluate AI application value

Identify where AI can create meaningful advantages.

2.
Map severity of bottlenecks

Prioritize pain points based on complexity, time impact, and iteration burden.

3.
Decide where to apply AI

Select use-cases where AI is both valuable and addresses bottlenecks.

Where can AI create a meaningful value?

1. Evaluate AI application value

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Select use-cases where AI is both valuable and addresses bottlenecks.

Lux's Application Value Framework

Automation Value
AI reduces manual effort, speeds up repetitive work, and increases throughput.

Knowledge Value
AI helps teams learn something they could not easily see on their own.

High

Knowledge value

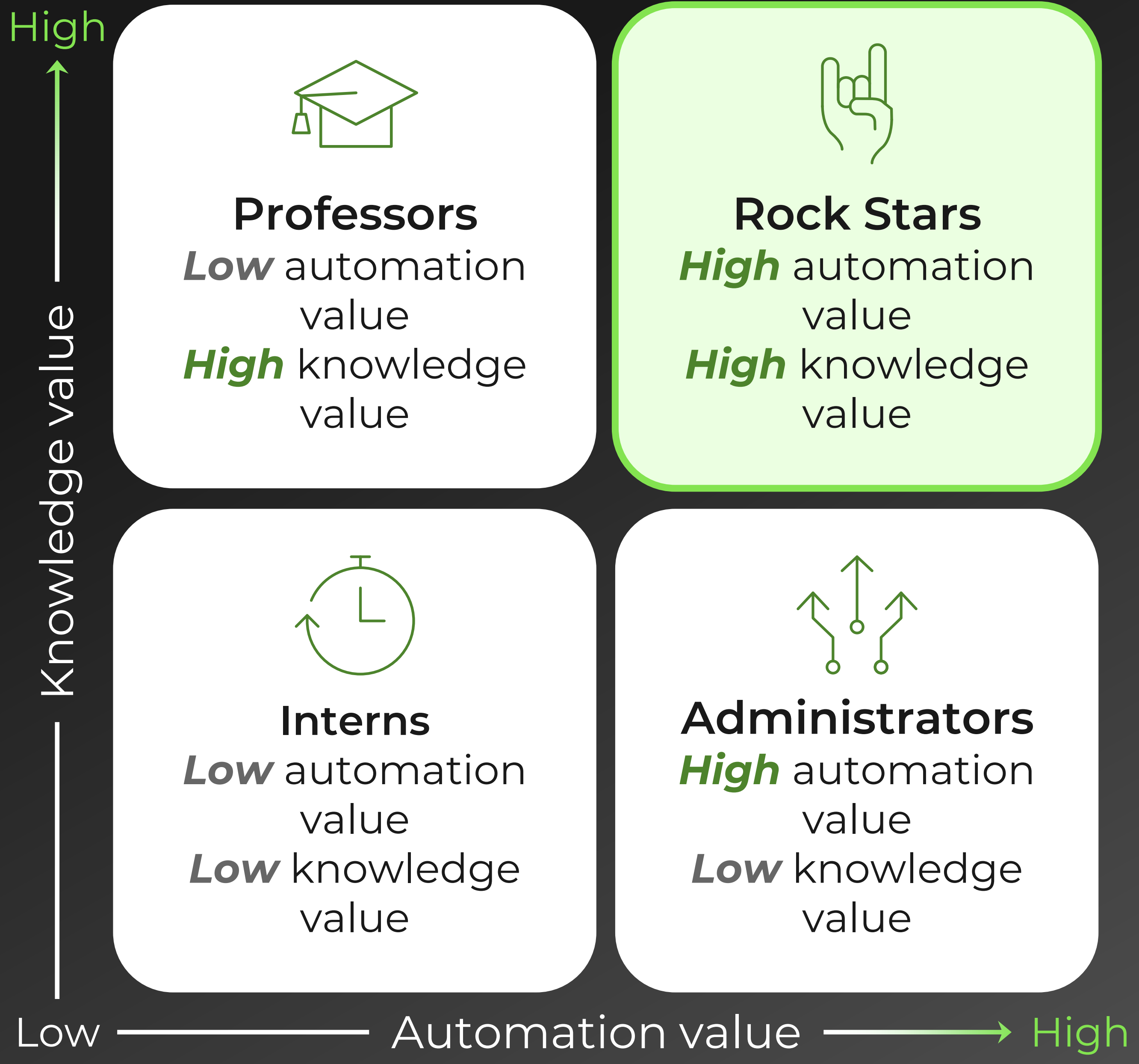
Knowledge value: High	**Professors** *Low* automation value *High* knowledge value	**Rock Stars** *High* automation value *High* knowledge value
Knowledge value: Low	**Interns** *Low* automation value *Low* knowledge value	**Administrators** *High* automation value *Low* knowledge value

Low — Automation value → High

Lux's Application Value Framework

Rock Stars

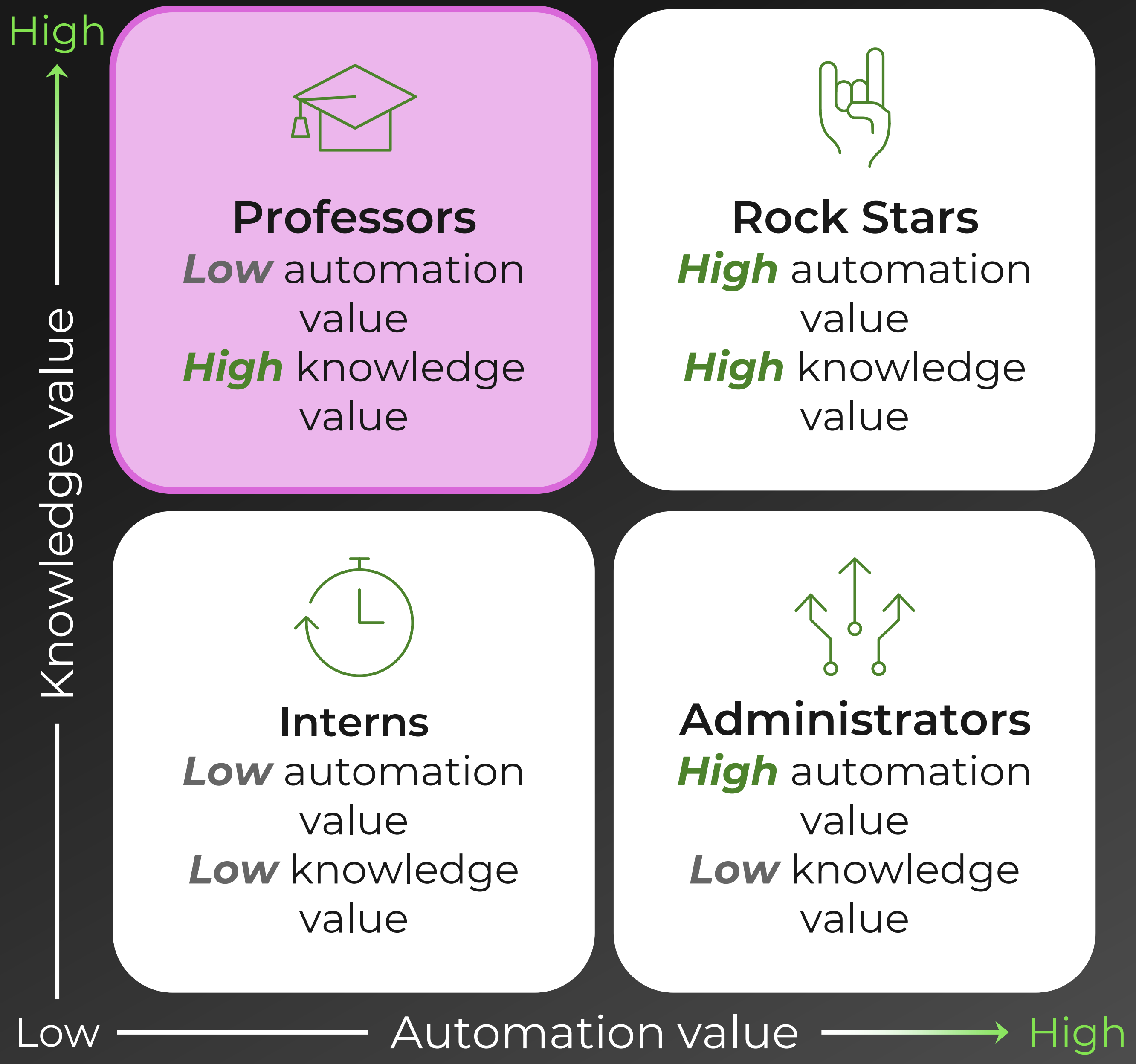
High-impact tasks where AI can accelerate repeated learning cycles and improve expert decisions.



Lux's Application Value Framework

Professors

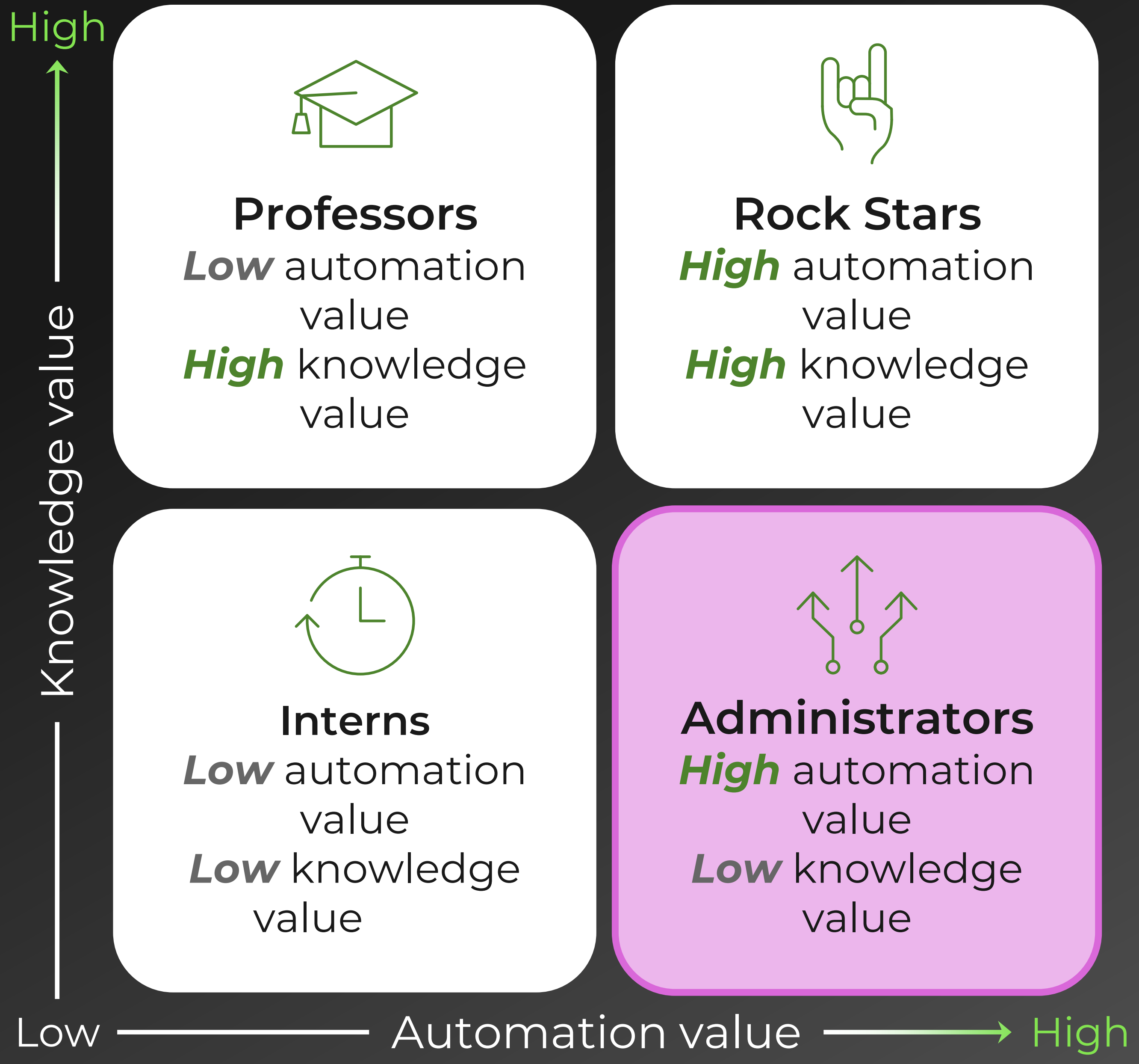
Expert-heavy tasks where AI helps surface patterns and options, but scientific judgment remains the limiting factor.



Lux's Application Value Framework

Administrators

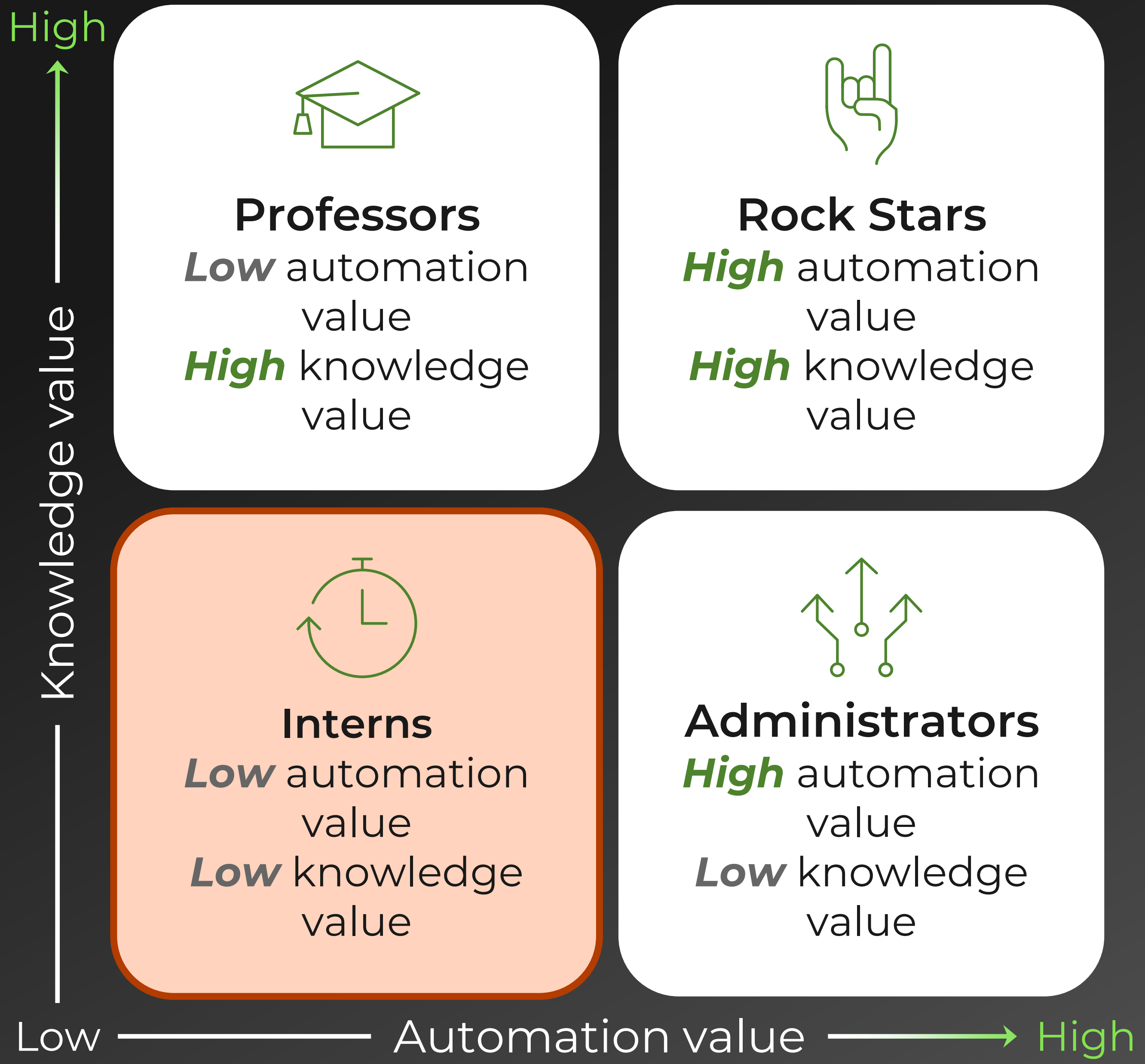
Repeatable workflows where AI and automation improve speed, consistency, and throughput, but do not fundamentally change material performance.



Lux's Application Value Framework

Interns

Low-leverage tasks where AI may save effort but is unlikely to change development timelines, costs, or success rates.



Where is the development workflow actually constrained?

1.
Evaluate AI application value

Identify where AI can create meaningful advantages.

2.
Map severity of bottlenecks

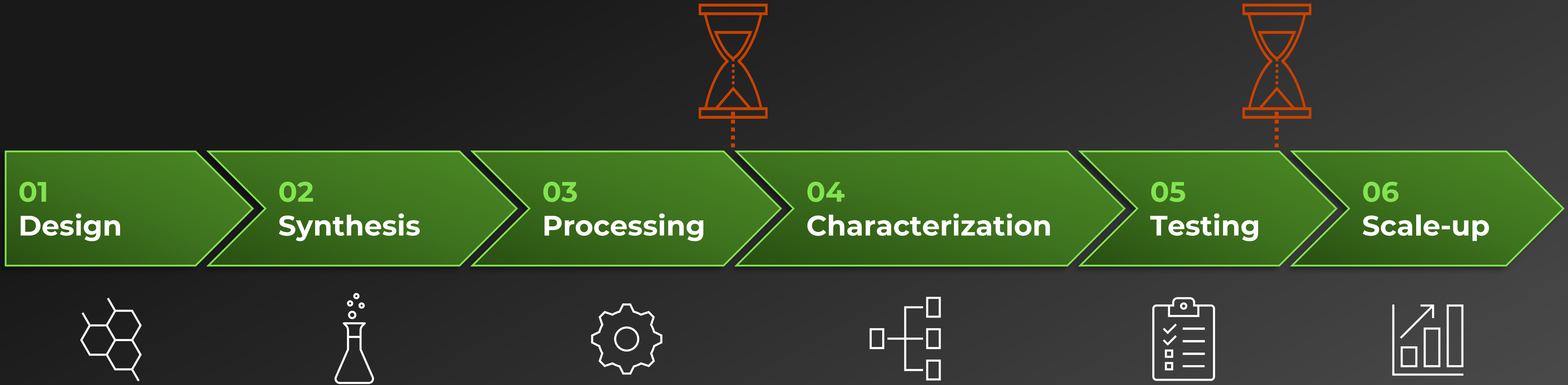
Prioritize pain points based on complexity, time impact, and iteration burden.

3.
Decide where to apply AI

Select use-cases where AI is both valuable and addresses bottlenecks.

Finding bottlenecks in materials development

A bottleneck is a step or sub-step or task that materially **slows progress**, **increases cost**, or **raises failure risk** in the development cycle.



3 critical factors to assign bottleneck severity

Technical complexity
How difficult the task is from a scientific and engineering standpoint.

Time impact
How strongly delays in the task affect the overall development timeline.

Iteration burden
How much effort, cost, and infrastructure are required to repeat and improve the task.

01 Design

02 Synthesis

03 Processing

04 Characterization

05 Testing

06 Scale-up

Bottleneck severity ranges from low to high

Low
Limited constraint with minor impact on speed, cost, or development outcomes.

Medium
Moderate constraint that creates delays or rework but does not consistently block progress.

High
Critical constraint that significantly slows development, increases cost, or raises failure risk.

01 Design

02 Synthesis

03 Processing

04 Characterization

05 Testing

06 Scale-up

Example: Battery Electrodes

01 **Design** → 02 **Synthesis** → 03 **Processing** → 04 **Characterization** → 05 **Testing** → 06 **Scale-up**

Low	Medium	Medium	Medium	Medium	High
Multi-objective design goals	Require strict process control	High-dimensional slurry formulation	Linking structure to degradation	Cycle life and rate performance testing	Complex systems integration
Complex electro-chemistry	Thermal / process window sensitivity	Achieving uniform slurry dispersion	3D electrode structure characterization	Long cycle life testing	Multiparameter process control
	Batch-to-batch variability	Multiparameter production optimization	Cycle life testing (time intensive)	Failure mode and safety validation	Complex integration across the supply chain

We conducted a comprehensive bottleneck analysis

ANALYSIS: MATERIAL BOTTLENECK

Bottlenecks and their severity vary across materials (1/3)

Steps	Sub-steps/tasks	Commodity polymers	PFAS Alternative	High entropy alloys
Design	Monomer/molecule selection	Limited design space	Complex chemistry	Huge design space
	Structure/system design	Multiscale and multi-physics modelling	Surface prediction is weak	Phase prediction limitation
Synthesis	Material preparation	Hard to maintain purity	Complex synthesis routes	High temperature processing
	Process control	Process control variation	Reaction condition sensitivity	Thermal process control
	Yield optimization	Incremental improvement in performance	Low yield due to multistep process	Defects affect usable yield
Formulation / Processing	Component selection	Large additive space	Multi-objective trade-off	NA
	Mixing/structuring	Dispersion quality control	Application parameters control	NA
	Process tuning	Process property coupling	Process control optimization	NA
Characterization	Structural/molecular	Standardized testing	Functional group identification	Phase identification difficult
	Morphology/surface	Linking morphology to properties	Surface heterogeneity detection	Complex grain structure and defects
	Property measurement	Standard tests at scale	Multi-condition performance testing	High-temperature testing
Testing	Performance testing	Application specific variable testing	Multi-condition performance benchmarking	Extreme conditions testing
	Stability/durability	Lengthy aging tests	Environmental durability testing	Long-duration stability testing
	Specialized validation	Application specific tests costly	Stringent regulatory testing	Limited specialized validation
Scale-up / Manufacturing	Process scale-up	Process efficiency and cost	Property variations at scale	Microstructure control difficult
	Process optimization	Incremental improvements in performance	Balance cost, compliance, and performance	Limited expertise
	Manufacturing integration	Mature but needs consistency	Must fit with current manufacturing	Limited industrial infrastructure

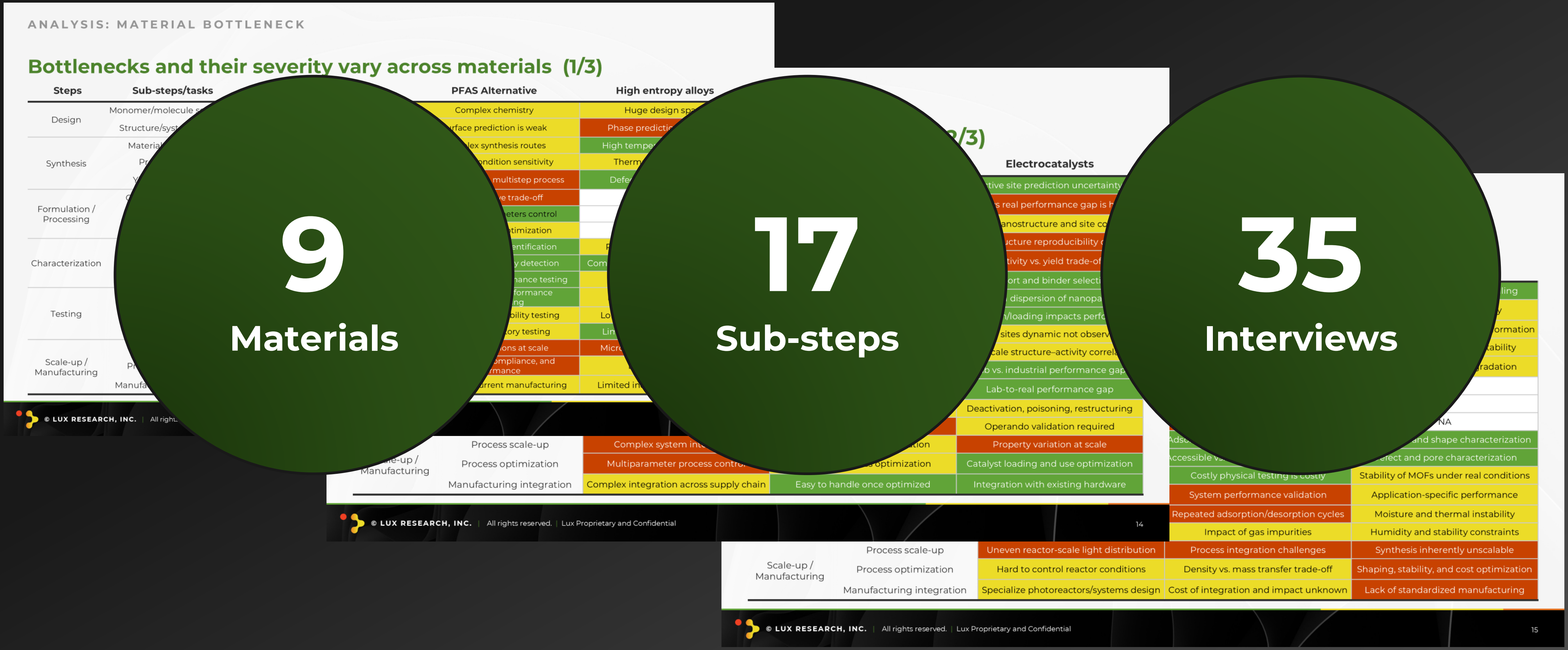
ross materials (2/3)

		Battery electrolytes	Electrocatalysts
		Interfacial compatibility uncertainty	Active site prediction uncertainty
		Interfacial chemistry modelling is poor	DFT vs real performance gap is high
		Strict contamination control	Hard nanostructure and site control
		Manufacturing environmental control	Nanostructure reproducibility control
		Contamination-induced rejection	Activity vs. yield trade-off
		Complex solvent–salt–additive match	Huge support and binder selection space
		aintain purity and avoid contamination	Uniform dispersion of nanoparticles
		Stability-essential process	Deposition/loading impacts performance
		Capturing interfacial chemical states	Active sites dynamic not observable
		Challenging at scale and in real time	Nanoscale structure–activity correlation
		Safety and stability characterization	Lab vs. industrial performance gap
		System-level performance validation	Lab-to-real performance gap
		Chemical and electrochemical stability	Deactivation, poisoning, restructuring
		Safety validation testing	Operando validation required
Scale-up / Manufacturing	Process scale-up	Complex system integration	Hard to control contamination	Property variation at scale
	Process optimization	Multiparameter process control	Chemical process optimization	Catalyst loading and use optimization
	Manufacturing integration	Complex integration across supply chain	Easy to handle once optimized	Integration with existing hardware

ross materials (3/3)

			Carbon sorbents	MOFs
			Complex surface chemistry modelling	Complex performance modelling
			Performance gap in modelling	Synthesis unpredictability
			Uniform functional group distribution	Hard to reproducible structure formation
			Maintain surface chemistry consistency	Crystallization process instability
			Functionalization efficiency limits	Scale-sensitive yield degradation
			Binder-performance trade-off	NA
			Hard to maintain pore accessibility	NA
			Pellet density vs.. performance trade-off	NA
			dsorption sites measurement challenge	Crystallinity and shape characterization
			ccessible vs. total porosity measurement	Defect and pore characterization
			Costly physical testing is costly	Stability of MOFs under real conditions
			System performance validation	Application-specific performance
			Repeated adsorption/desorption cycles	Moisture and thermal instability
			Impact of gas impurities	Humidity and stability constraints
Scale-up / Manufacturing	Process scale-up	Uneven reactor-scale light distribution	Process integration challenges	Synthesis inherently unscalable
	Process optimization	Hard to control reactor conditions	Density vs. mass transfer trade-off	Shaping, stability, and cost optimization
	Manufacturing integration	Specialize photoreactors/systems design	Cost of integration and impact unknown	Lack of standardized manufacturing

We conducted a comprehensive bottleneck analysis



A 3-step process for prioritizing AI opportunities

1. Evaluate AI application value

Identify where AI can create meaningful advantages.

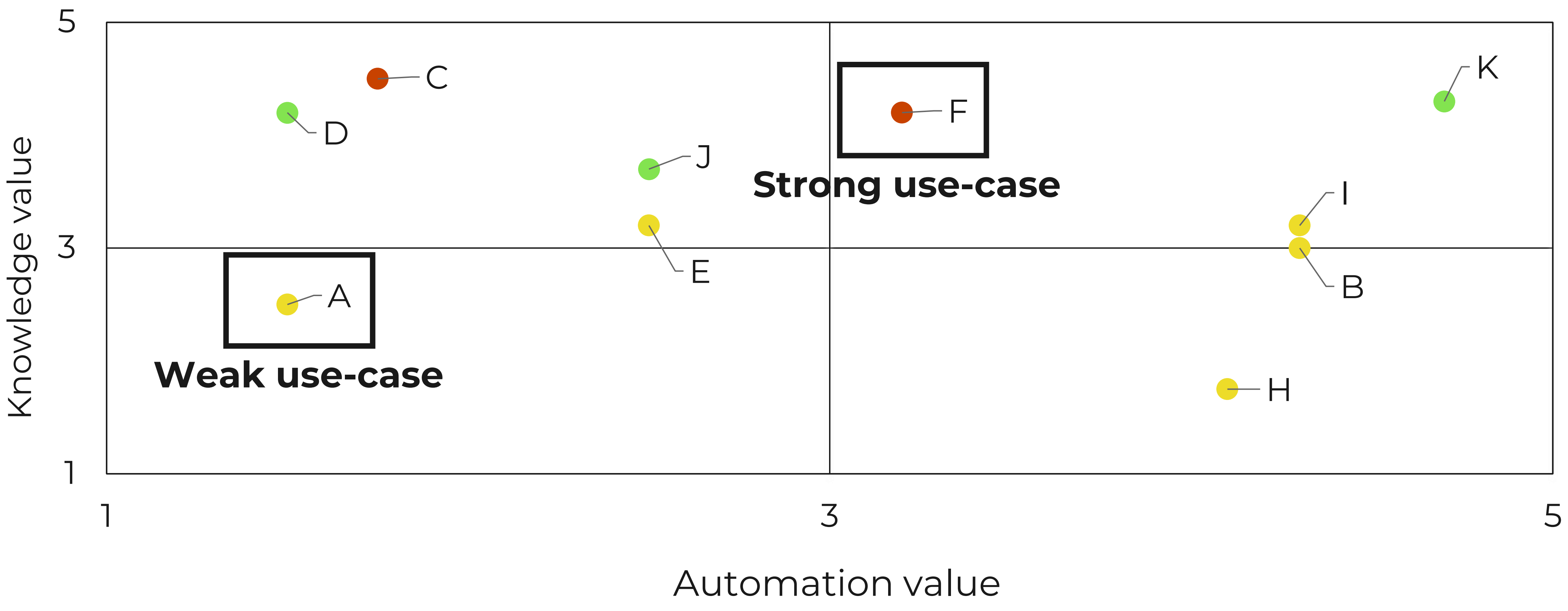
2. Map severity of bottlenecks

Prioritize pain points based on complexity, time impact, and iteration burden.

3. Decide where to apply AI

Select use-cases where AI is both valuable and addresses bottlenecks.

Selecting use-cases where AI is valuable and addresses bottlenecks



Agenda

01 | Evaluating AI’s value across the materials development workflow

02 | **Diving deep into specific materials examples**

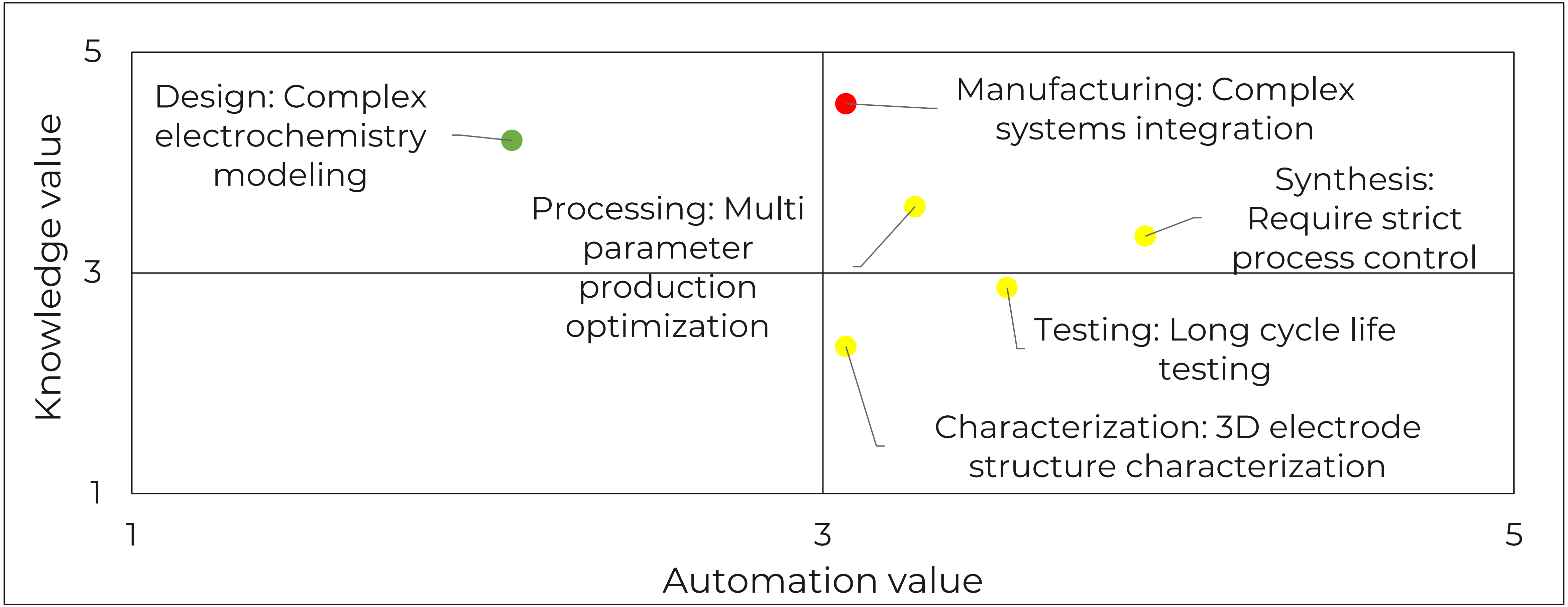
03 | Looking ahead for AI-enabled materials R&D

Battery Electrode Materials

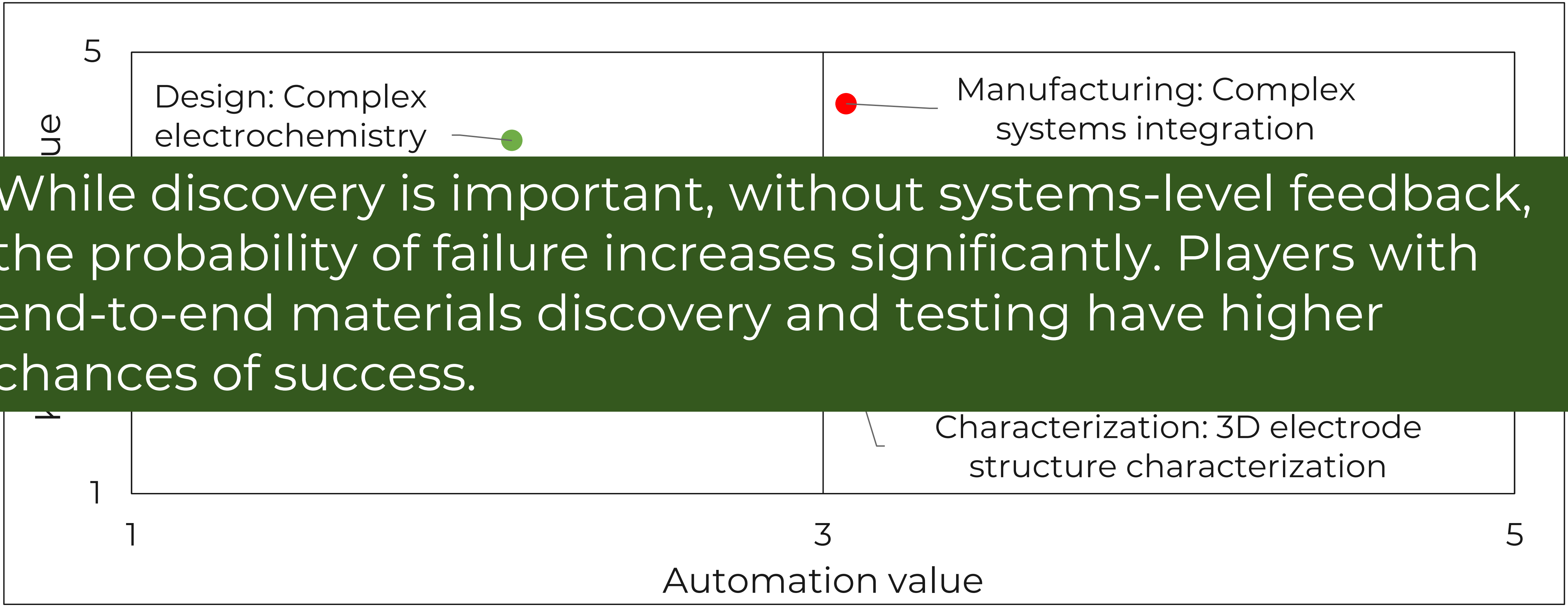
Battery electrode bottleneck identification

01 Design	02 Synthesis	03 Processing	04 Characterization	05 Testing	06 Scale-up
Low	**Medium**	**Medium**	**Medium**	**Medium**	**High**
Multi-objective design goals	Require strict process control	High-dimensional slurry formulation	Linking structure to degradation	Cycle life and rate performance testing	Complex systems integration
Complex electro-chemistry	Thermal / process window sensitivity	Achieving uniform slurry dispersion	3D electrode structure characterization	Long cycle life testing	Multiparameter process control
	Batch-to-batch variability	Multiparameter production optimization	Cycle life testing (time intensive)	Failure mode and safety validation	Complex integration across the supply chain

Selecting AI use-cases for battery electrode development



Selecting AI use-cases for battery electrode development



While discovery is important, without systems-level feedback, the probability of failure increases significantly. Players with end-to-end materials discovery and testing have higher chances of success.

CASE STUDY

Wildcat Discovery

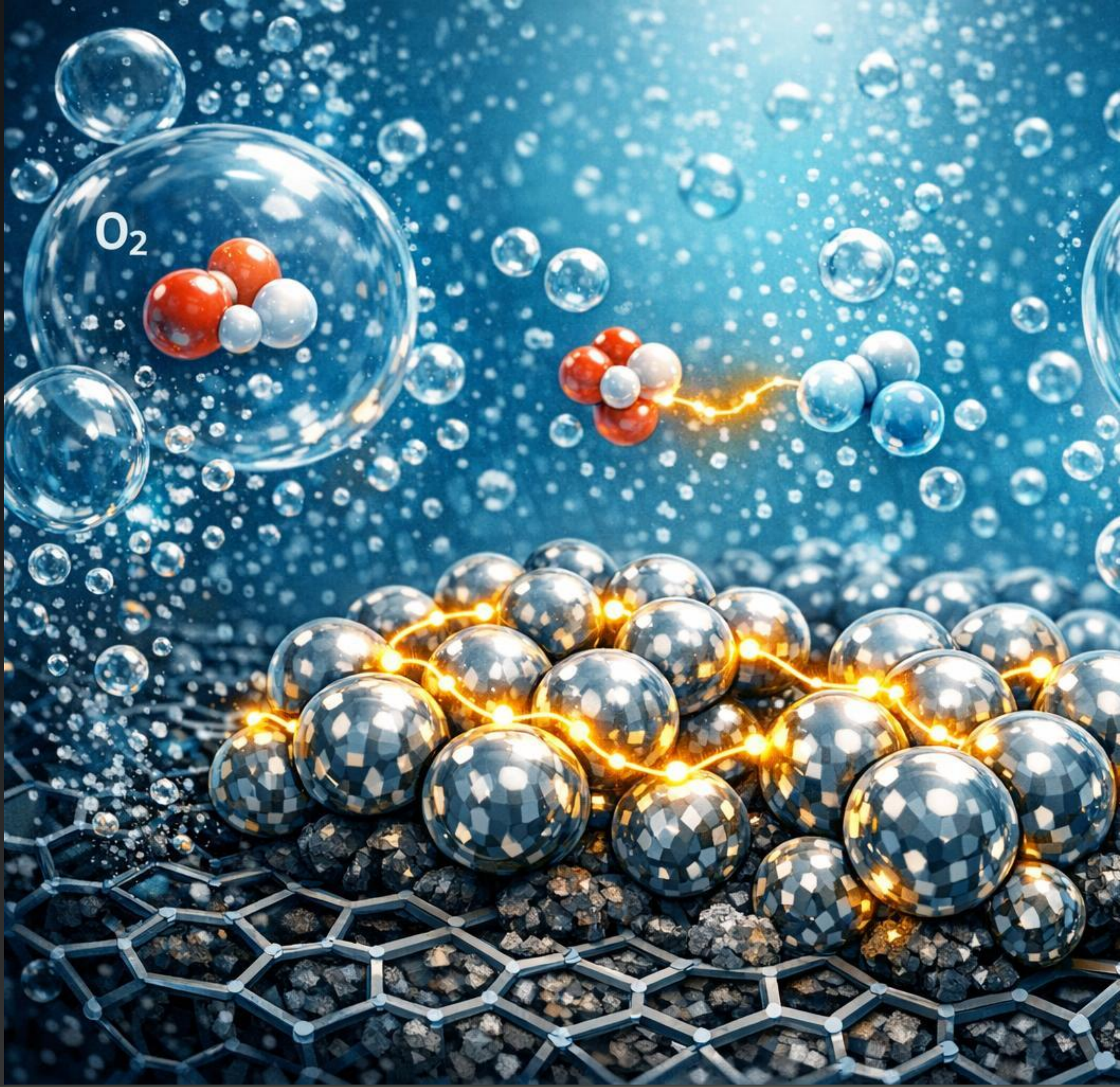
- Used AI-assisted cathode materials discovery and high-throughput experimentation to accelerate early stage battery materials development.
- Raised more than USD 190 million to build an AI-enabled cathode discovery platform but was later acquired by Holyvolt for EUR 63.1 million

LUX TAKE

Use AI to accelerate early battery materials discovery but prioritize systems-level validation and manufacturing readiness to convert promising candidates into commercial products.

Wildcat Discovery Technologies

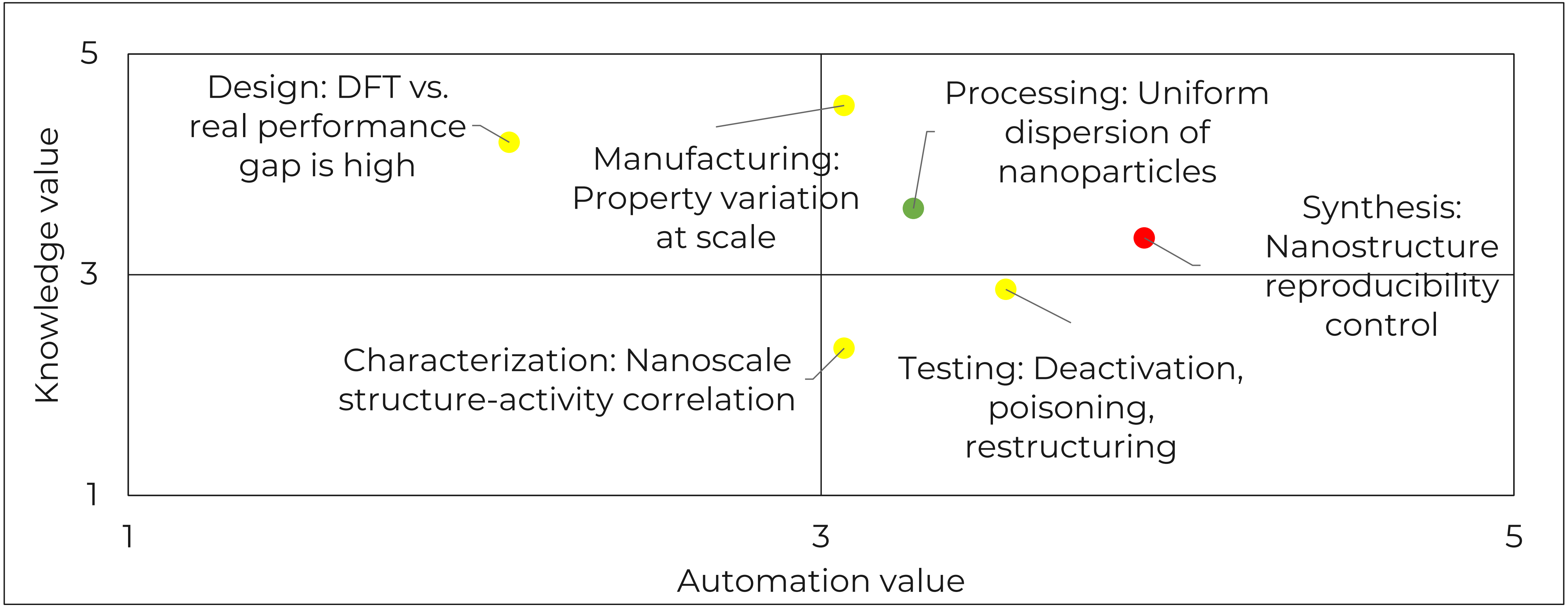
Electrocatalysis Materials



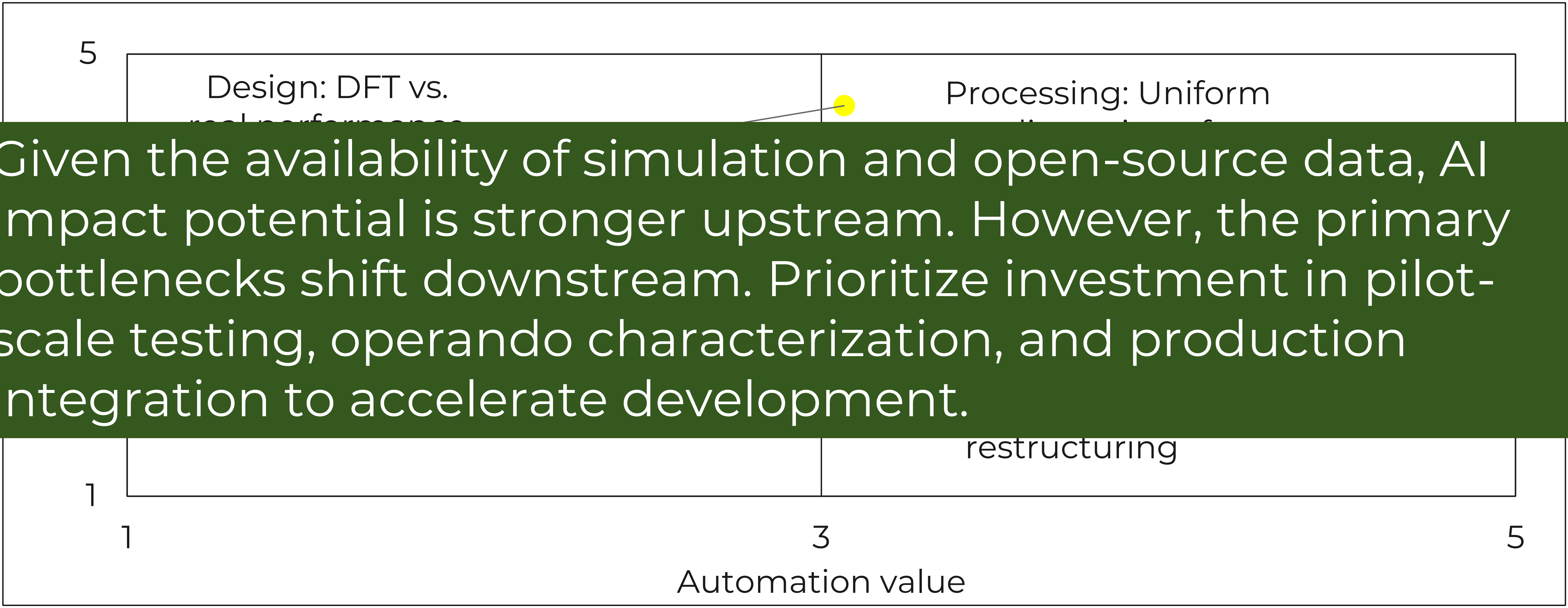
Electrocatalyst bottleneck identification

01 Design	02 Synthesis	03 Processing	04 Characterization	05 Testing	06 Scale-up
Medium	**High**	**Low**	**Medium**	**Medium**	**Medium**
Active site prediction uncertainty	Hard nanostructure and site control	Huge support and binder selection space	Active sites dynamic not observable	Lab to real performance gap	Property variation at scale
DFT vs. real performance gap is high	Nanostructure reproducibility control	Uniform dispersion of nanoparticles	Nanoscale structure-activity correlation	Deactivation, poisoning, restructuring	Catalyst loading and use optimization
	Activity versus yield tradeoff	Deposition and loading impacts performance	Lab vs. industrial performance gap	Operando validation required	Integration with existing hardware

Selecting AI use-cases for electrocatalyst development



Selecting AI use-cases for electrocatalyst development



Given the availability of simulation and open-source data, AI impact potential is stronger upstream. However, the primary bottlenecks shift downstream. Prioritize investment in pilot-scale testing, operando characterization, and production integration to accelerate development.

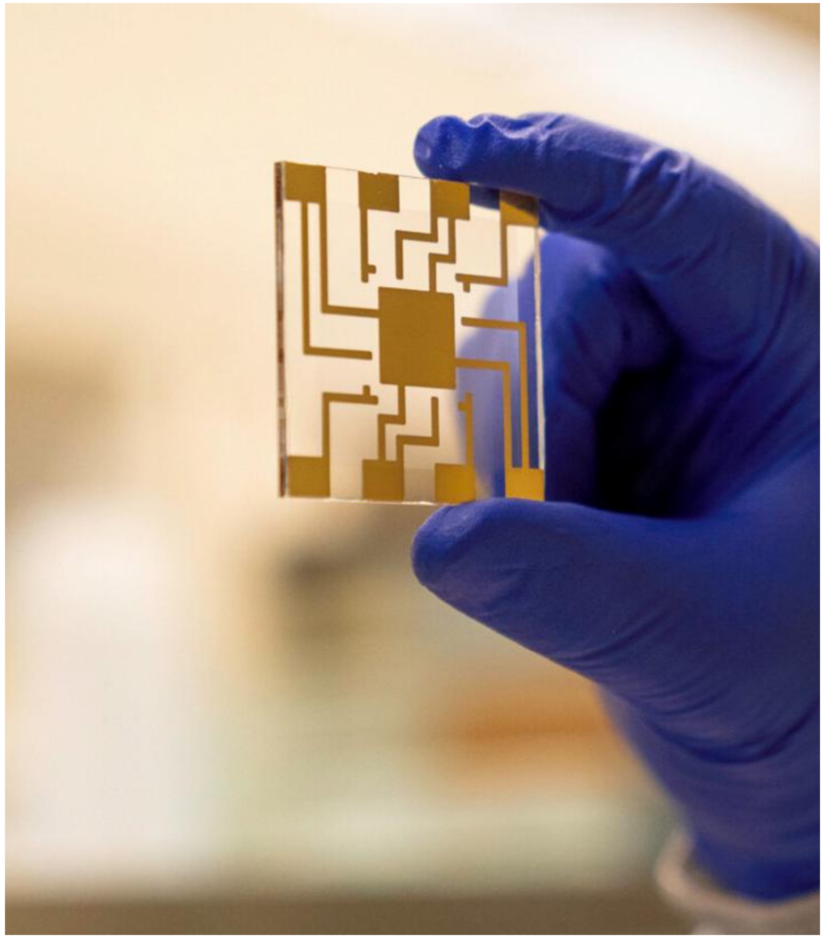
CASE STUDY

Mattiq

- Uses high-throughput experimentation and nanoscale lithographic methods to explore multi-metal catalyst combinations and generate proprietary experimental data.
- Developed a low-iridium catalyst using ruthenium oxide in collaboration with Heraeus, cutting iridium consumption by 75% and showing a pathway toward lower-cost electrolysis catalysts.

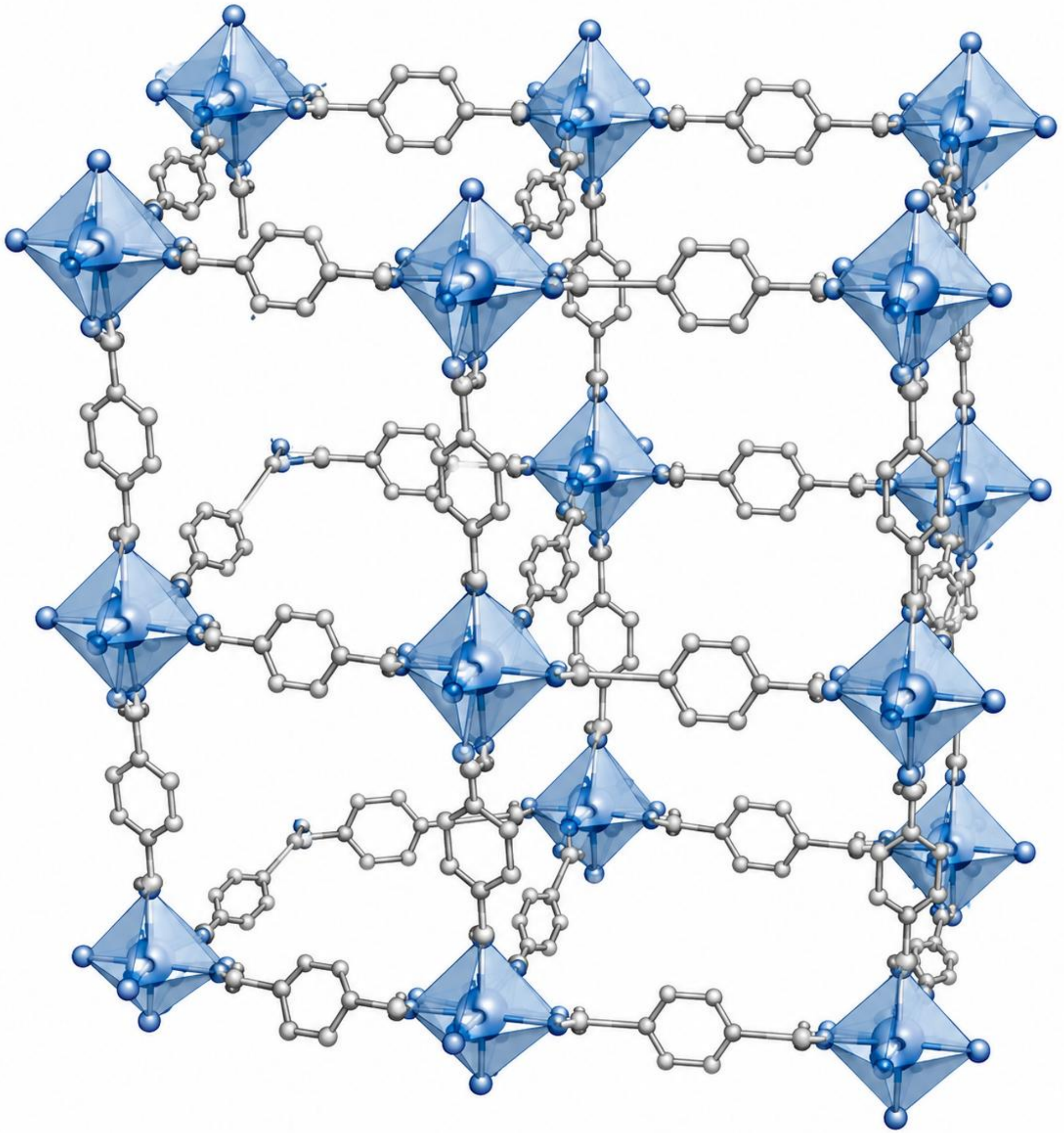
LUX TAKE

Prioritize building proprietary experimental feedback loops and validation capabilities, as these create more durable competitive advantage in catalyst AI than the model itself.



mattiq Heraeus

Metal Organic Frameworks (MOFs)

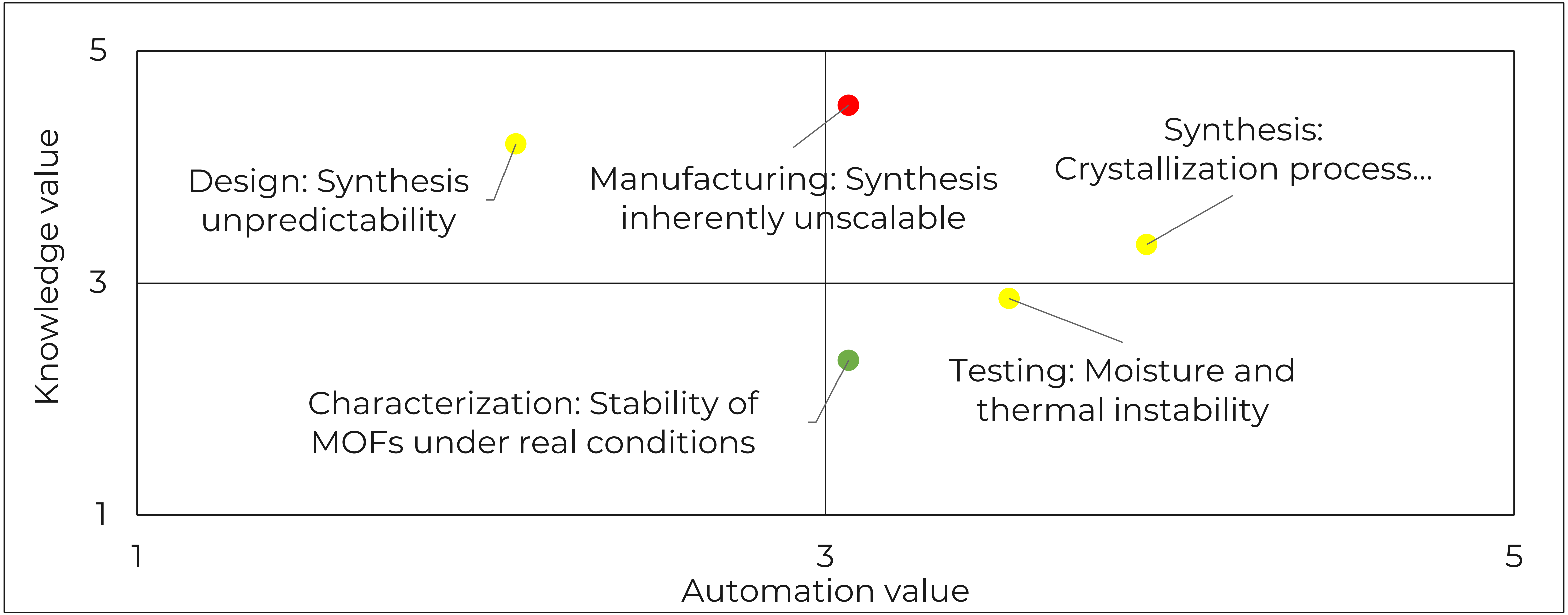


MOF bottleneck identification

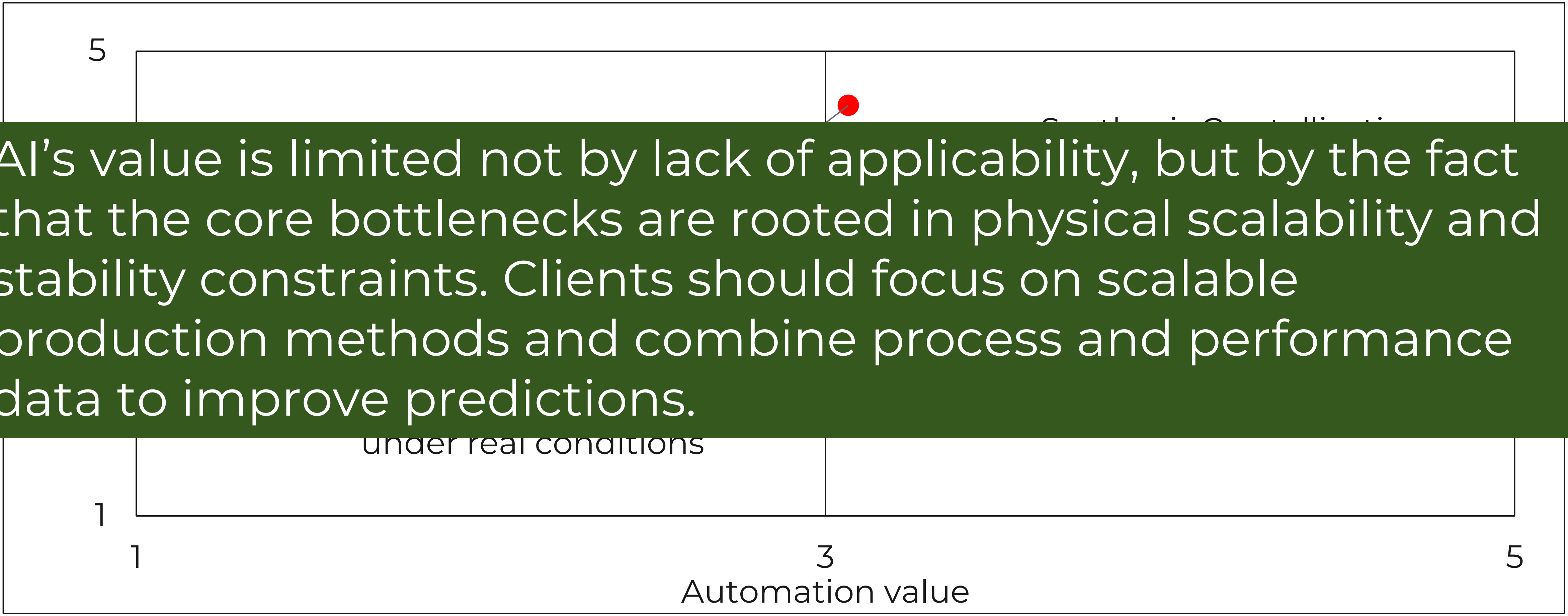
01 Design → **02 Synthesis** → **03 Processing** → **04 Characterization** → **05 Testing** → **06 Scale-up**

Medium	Medium	NA	Low	Medium	High
Complex performance modeling	Hard to reproduce structure formation	NA	Crystallinity and shape characterization	Application-specific performance	Synthesis inherently unscalable
Synthesis unpredictability	Crystallization process instability	NA	Defect and pore characterization	Moisture and thermal instability	Shaping, stability, and cost optimization
	Scale-sensitive yield degradation	NA	Stability of MOFs under real conditions	Humidity and stability constraints	Lack of standardized manufacturing

Selecting AI use-cases for MOF development



Selecting AI use-cases for MOF development



AI's value is limited not by lack of applicability, but by the fact that the core bottlenecks are rooted in physical scalability and stability constraints. Clients should focus on scalable production methods and combine process and performance data to improve predictions.

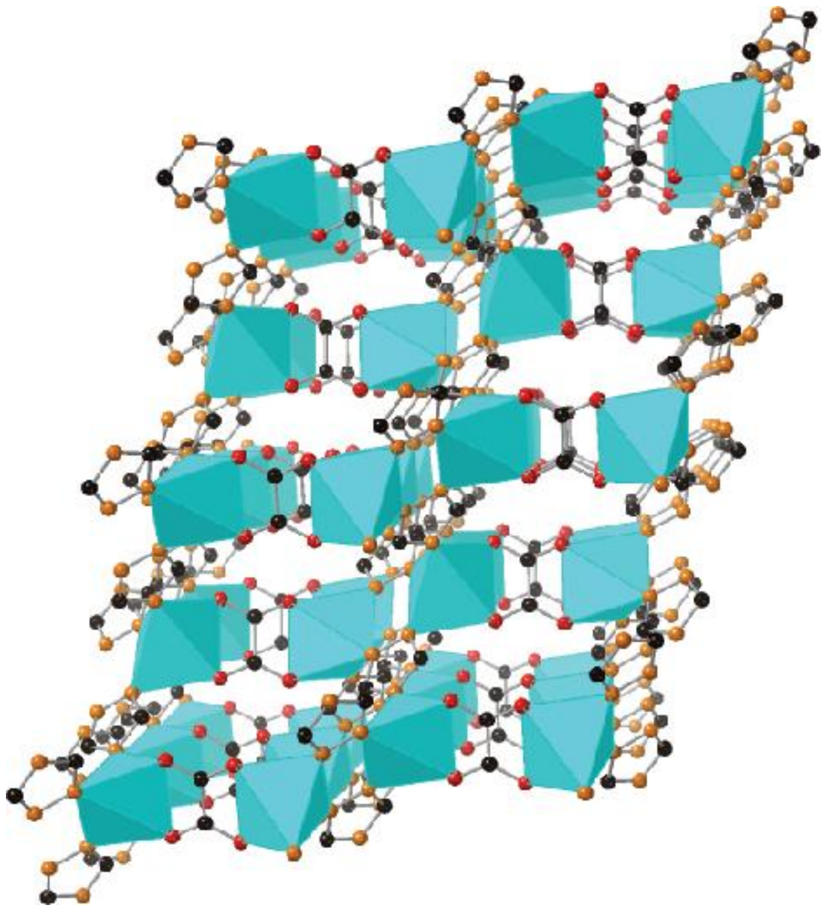
CASE STUDY

CuspAI

- Uses a multi-agent AI platform to generate new MOF structures and aims to combine generative discovery with self-driving laboratories.
- Has raised USD 130 million to date, aiming to build self-driving laboratories.

LUX TAKE

Use AI to accelerate MOF discovery, but do not let discovery outpace manufacturability.



Agenda

01 | Evaluating AI's value across the materials development workflow

02 | Diving deep into specific materials examples

03 | **Looking ahead for AI-enabled materials R&D**

Charting your AI for materials R&D roadmap

	Step 1	Step 2	Step 3
Use-case priorities	Map bottleneck severity and quadrant position before selecting any AI tool.	Select the use-case where AI value overlaps with a severe bottleneck.	Build closed-loop technical systems so AI improves each iteration.
Capability foundations	Standardize experimental, testing, and process data to build a data foundation.	Make AI part of scientist and engineer decision-making, not a standalone tool.	Integrate manufacturing from day one.

Adopting AI is not just a software decision

Use-case priorities	Map bottleneck severity and quadrant position before selecting any AI tool.	Select the use-case where AI value overlaps with a severe bottleneck.	Build closed-loop technical systems so AI improves each iteration.
Capability foundations	Standardize experimental, testing, and process data to build a data foundation.	Make AI part of scientist and engineer decision-making, not a standalone tool.	Integrate manufacturing from day one.

Adopting AI is not just a software decision

Map bottleneck severity

Select the use-case

Build closed-loop

AI adoption is not just a technology roadmap. It is a learning-systems roadmap.

Capability foundation

Standardize experimental, testing, and process data to build a data foundation.

Make AI part of scientist and engineer decision-making, not a standalone tool.

Integrate manufacturing from day one.

Key Takeaways

1

AI does not create value everywhere equally.

AI can support many parts of the materials development workflow, but its value depends on the task.

2

The biggest bottleneck is rarely where the AI hype is.

The public conversation often focuses on discovery, but that is not always the limiting step. Companies should start by asking where the development process is actually constrained.

3

Winning organizations combine AI, experimentation, and domain expertise in closed learning loops.

The organizations that win will be the ones that connect AI to experiments, workflows, and technical judgment so each cycle makes the next one smarter.

Lux Client Action Items

1 **Diagnose before you deploy.**

Map your material's bottlenecks and identify which workflow stage is genuinely rate limiting before selecting any AI tool.

2 **Prioritize one high-value use-case first.**

Pick one workflow where AI value overlaps with a severe bottleneck, then scale.

3 **Audit your data infrastructure.**

For each AI use-case under consideration, identify the specific training data set required. Focus on building a robust data pipeline with internal efforts or through collaborations.

4 **Build manufacturing integration from day one.**

Design AI programs to include manufacturability, process windows, cost, quality, and scale-up feedback from the beginning.

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