

2024

Innovation China Conference

创新中国研讨会

Shanghai, China | 29 April 2024

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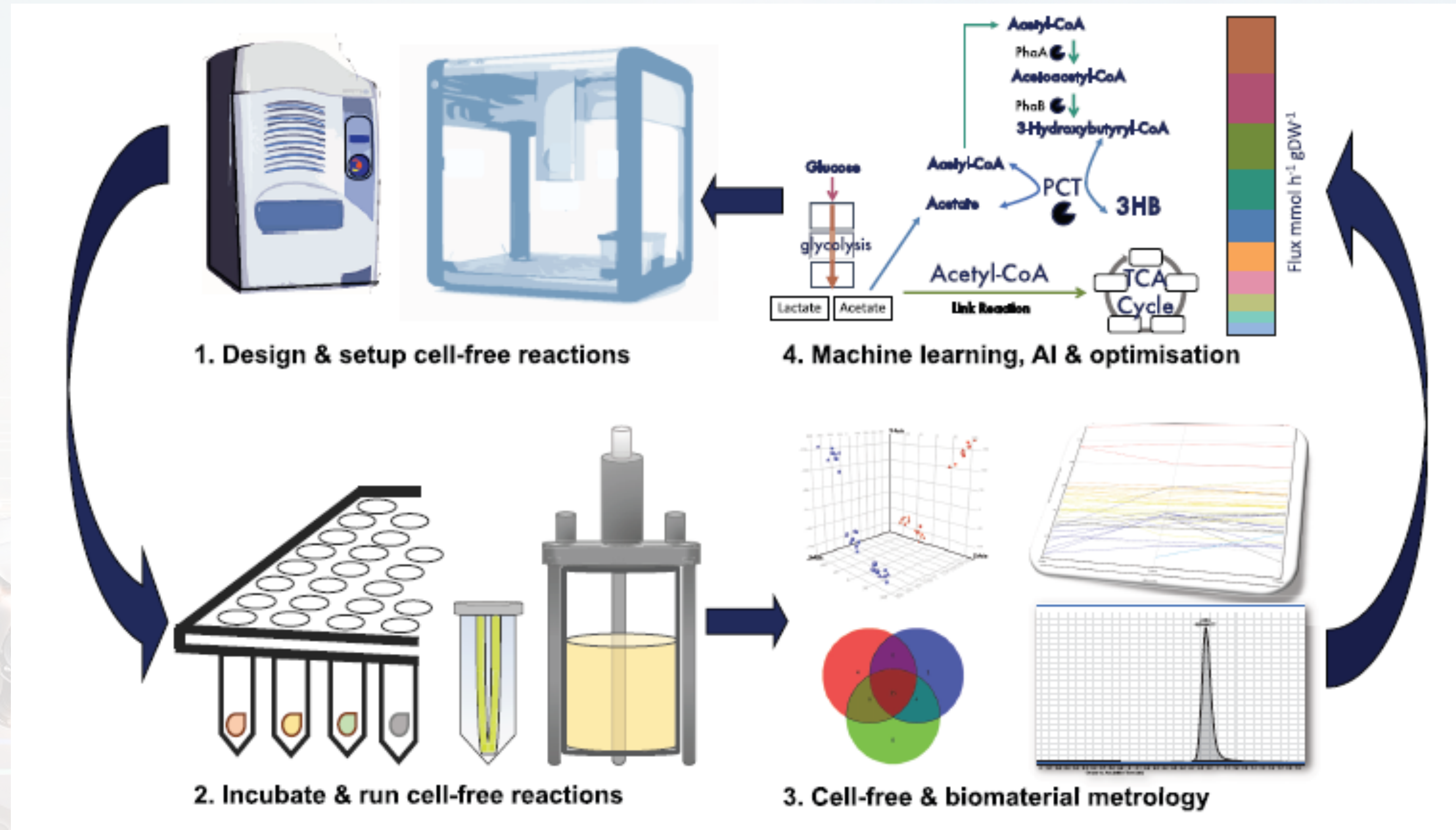
A.I.+

AI + Materials 材料 | AI + Industrials 工业 | AI + New Energy 新能源

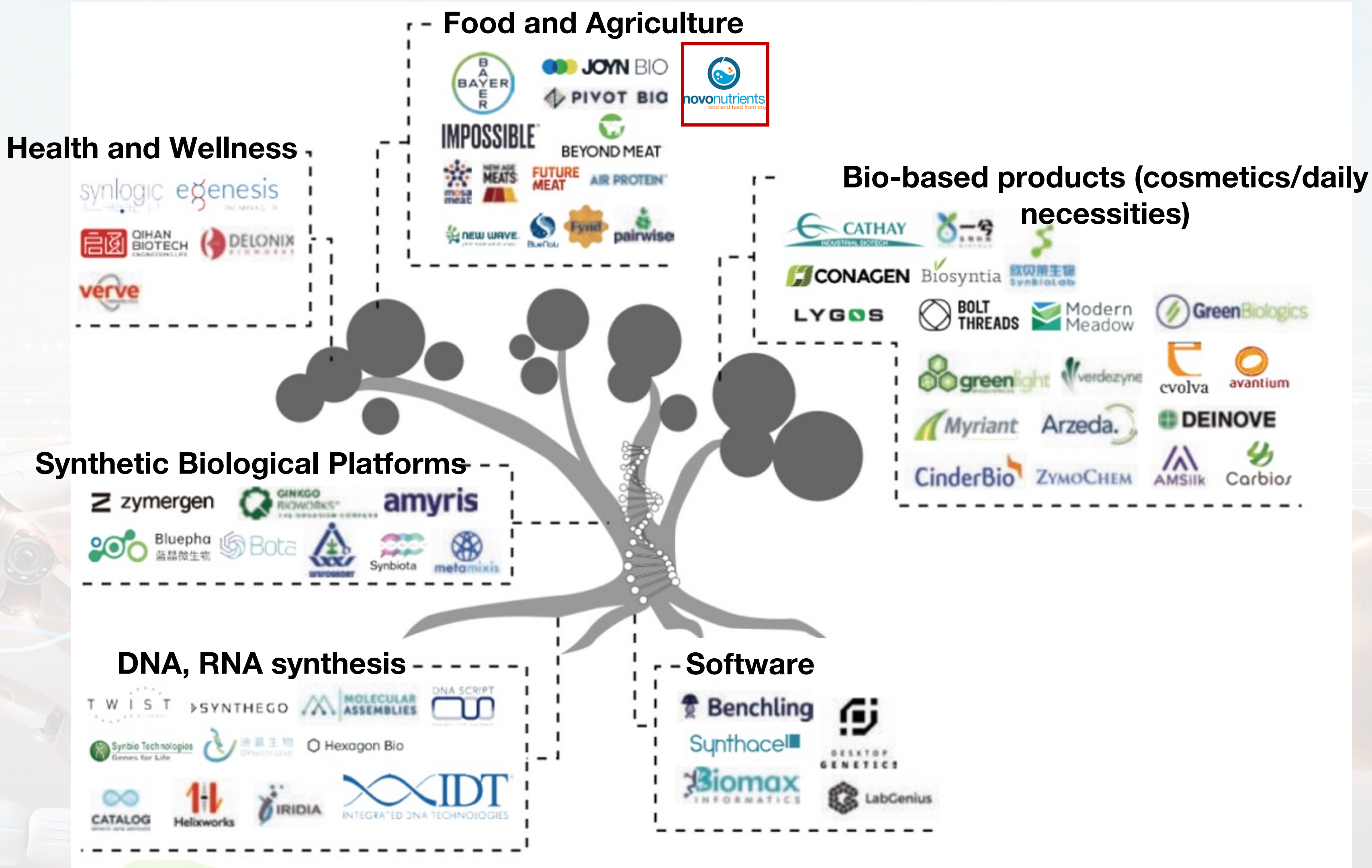
AI for Materials

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The Design > Build > Test > Learn cycle in synbio



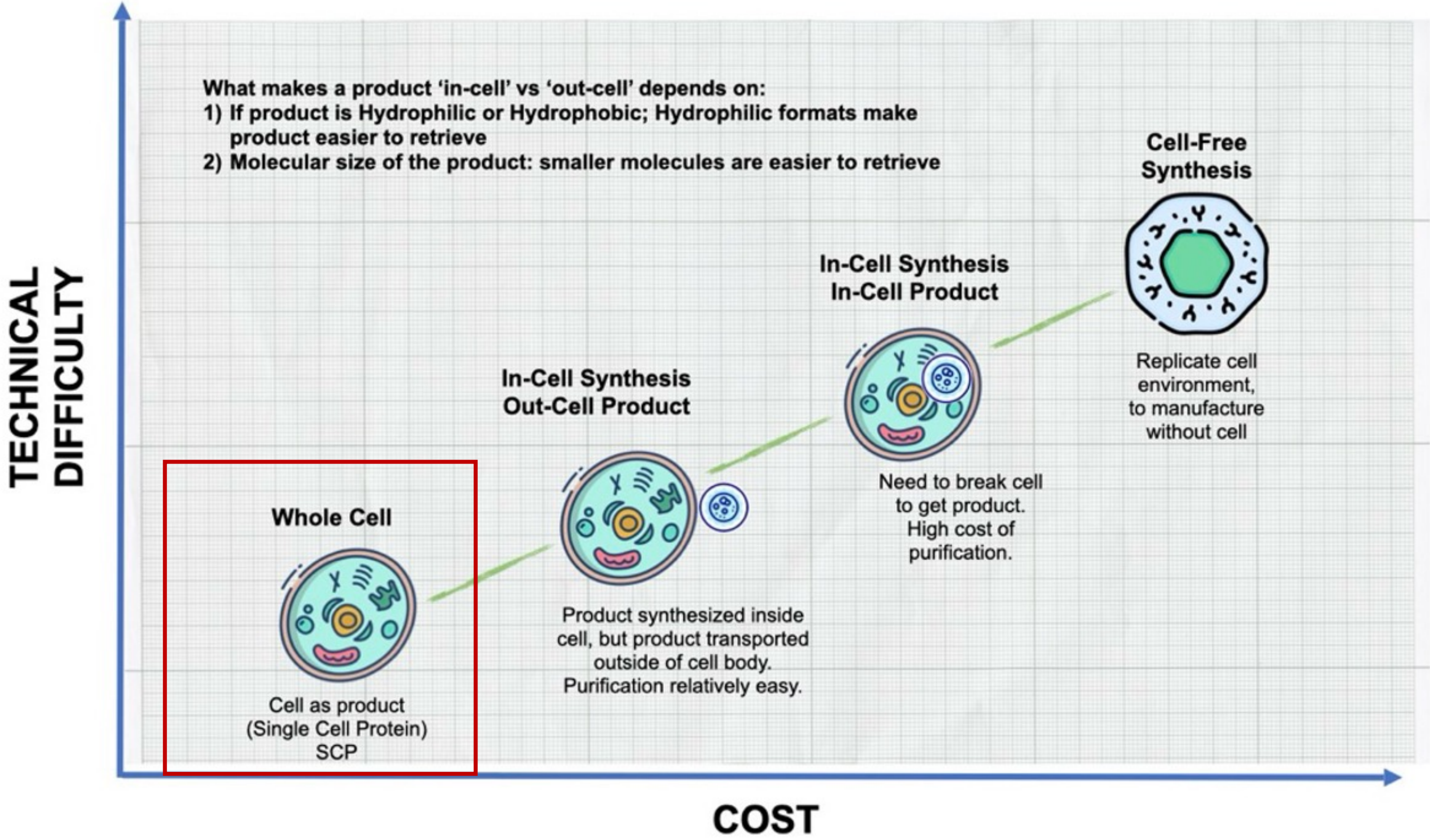
Synbio has many startups in the West



Synbio itself has levels of TRLs*

*Technology Readiness Level

The Synbio Era is coming: Full-Cell vs Cell-Free

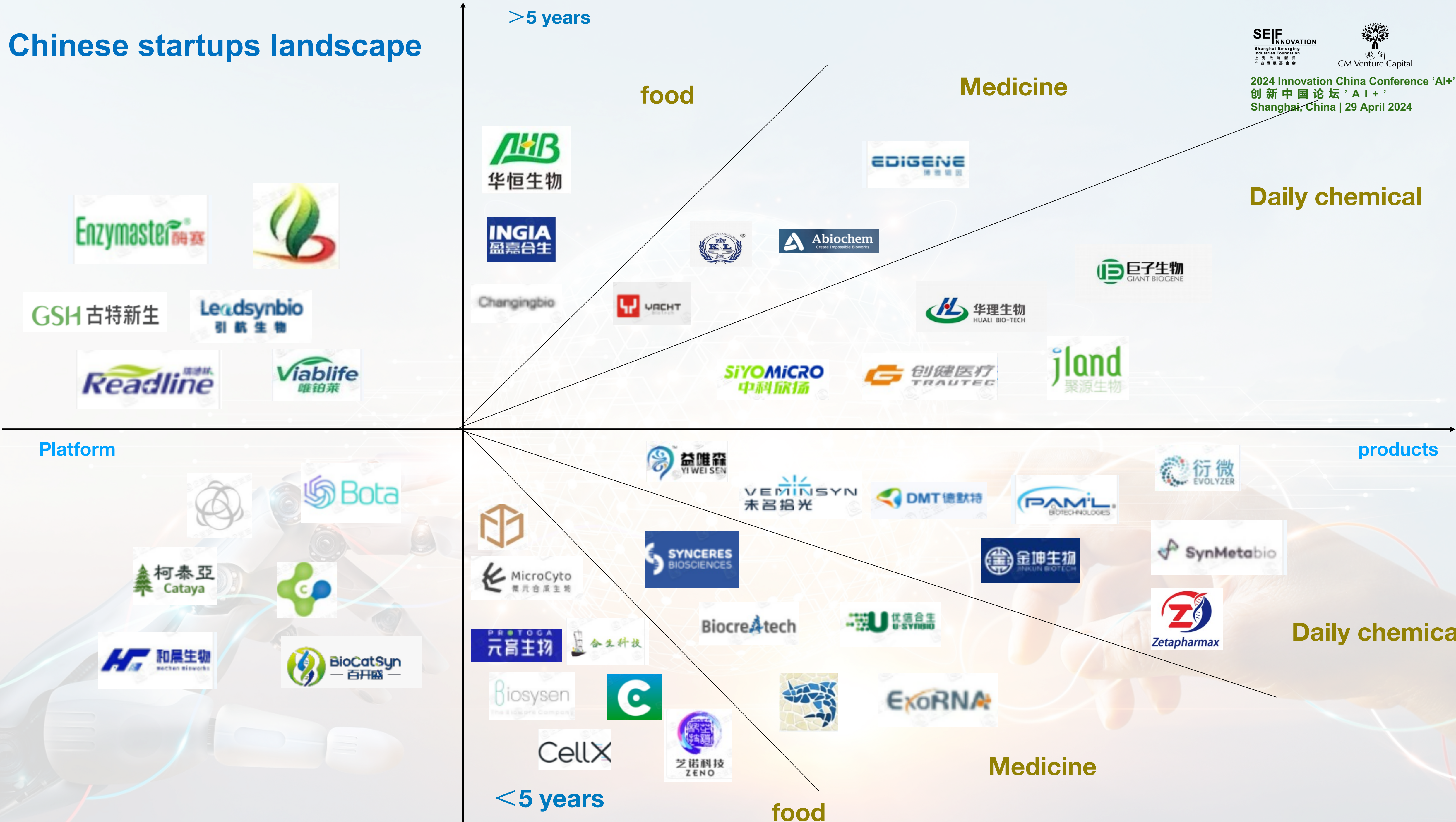


Chinese startups landscape

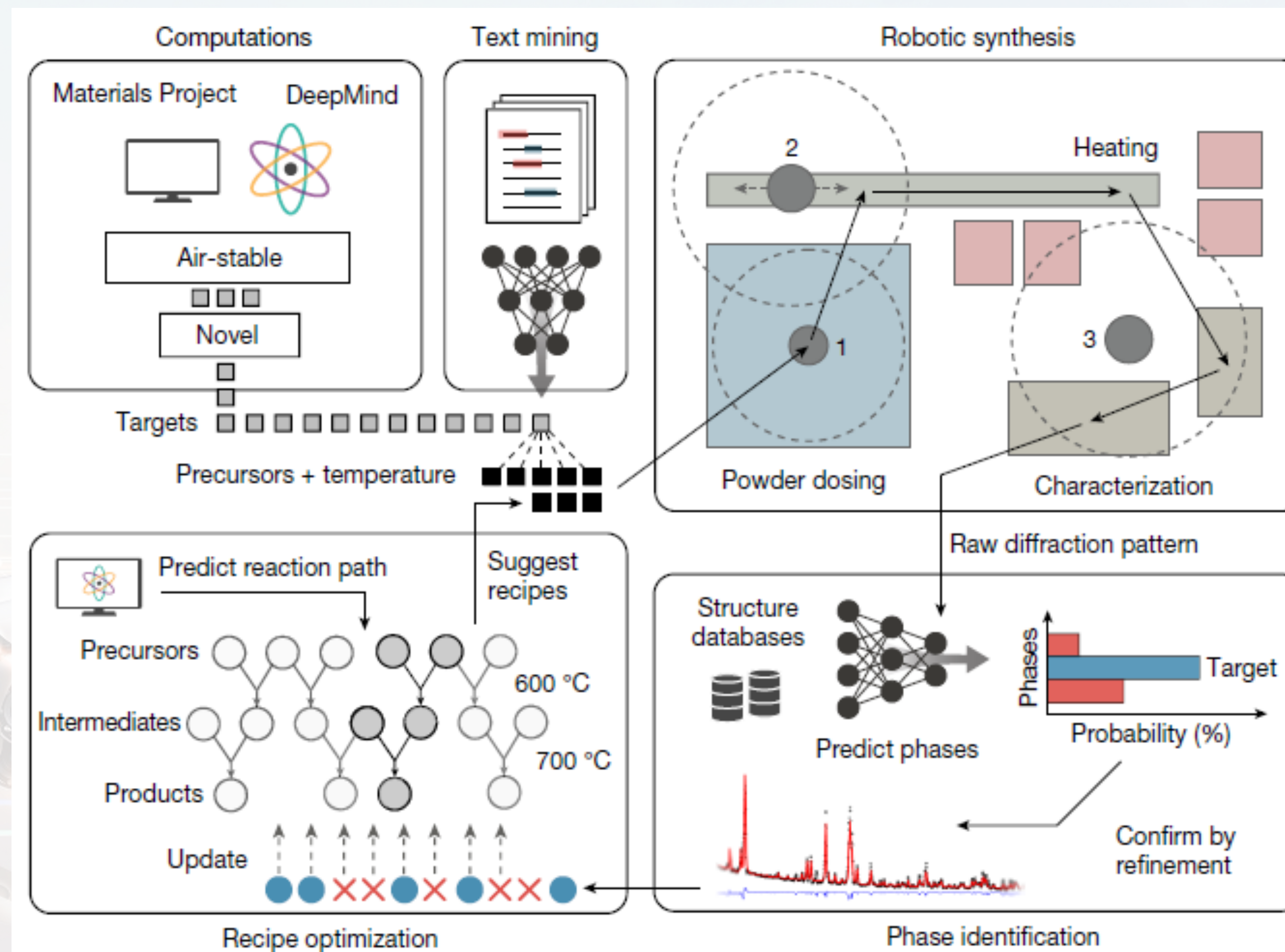
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2024 Innovation China Conference 'AI+'
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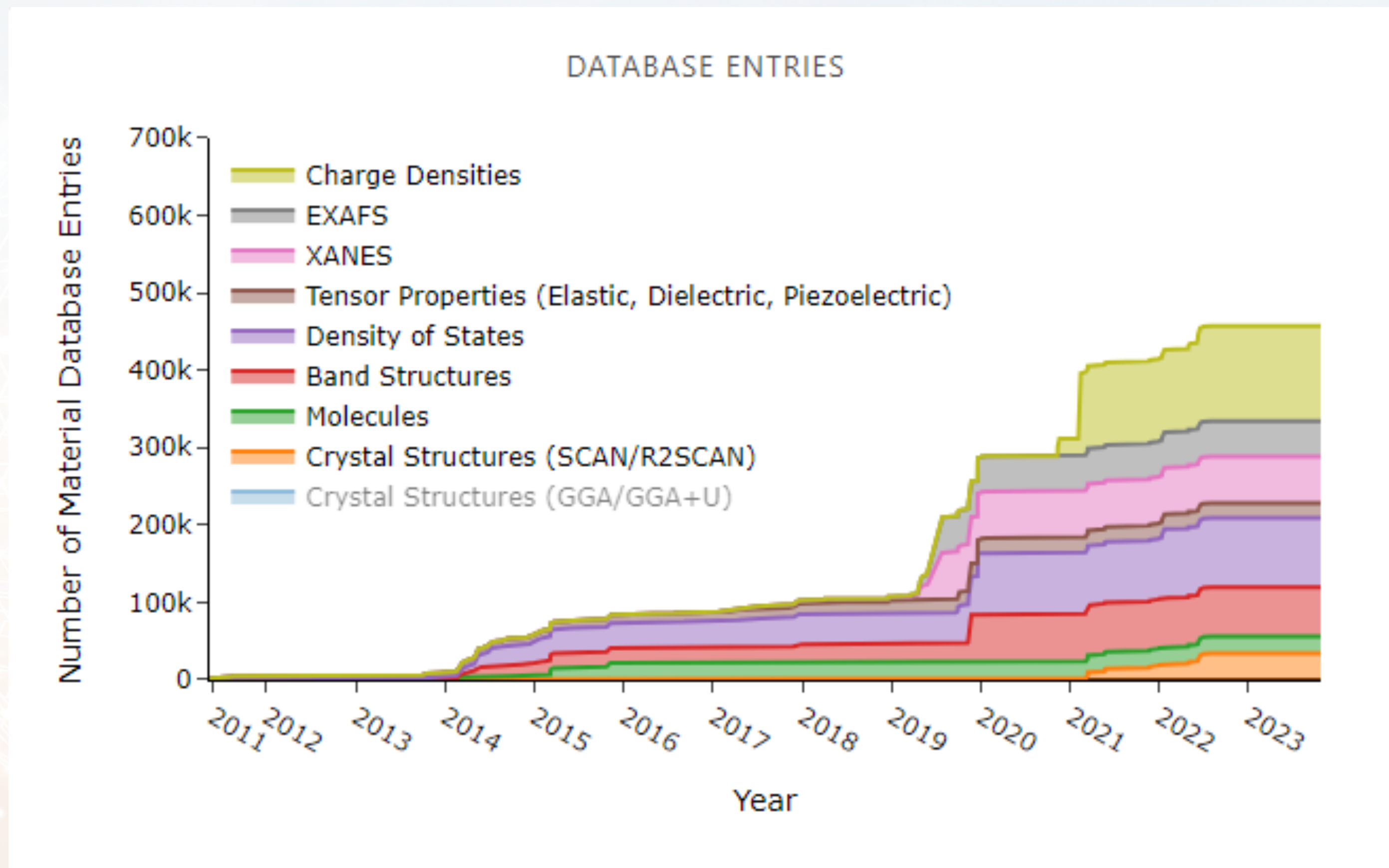


Materials discovery has similar Design > Build > Test > Learn cycle



Source: "An autonomous laboratory for the accelerated synthesis of novel materials", Nature Vol 624 December 7 2023

The Materials Project (US) started in 2011



But the discovery of new materials remains challenging



“...an order-of-magnitude expansion in stable materials known to humanity”

Artificial Intelligence Driving Materials Discovery? Perspective on the Article: Scaling Deep Learning for Materials Discovery

Anthony K. Cheetham* and Ram Seshadri*



Cite This: <https://doi.org/10.1021/acs.chemmater.4c00643>



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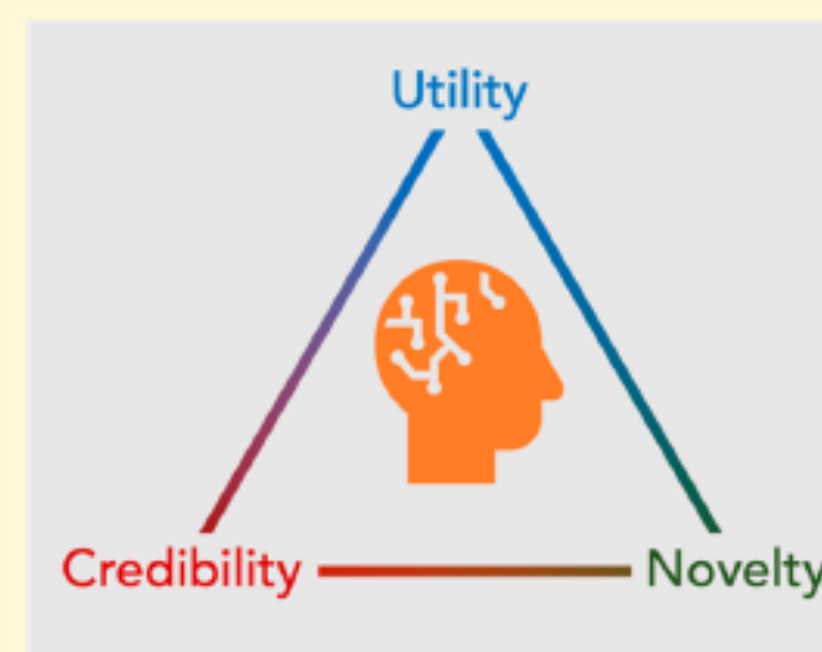


Metrics & More

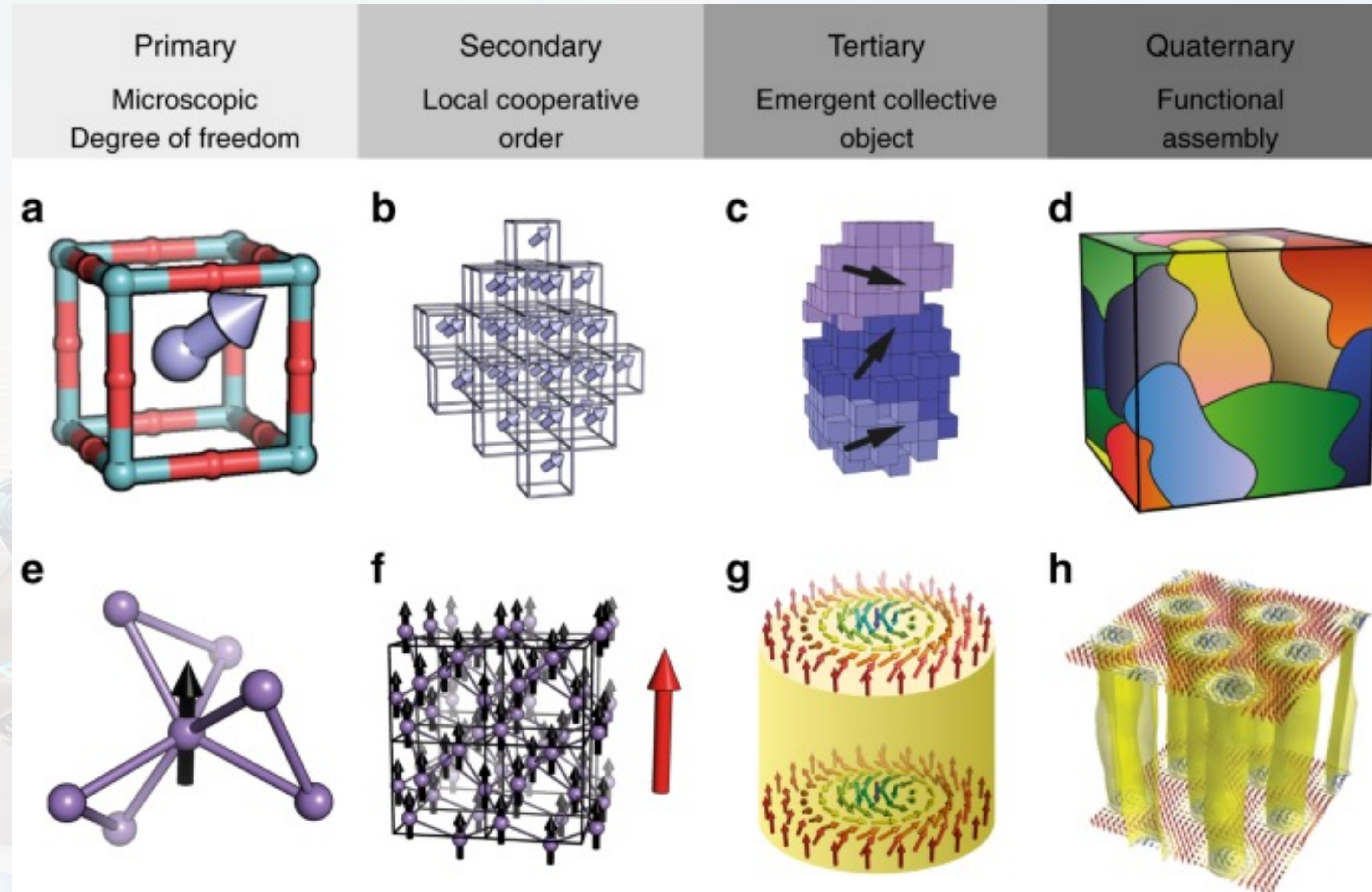


Article Recommendations

ABSTRACT: The discovery of new crystalline inorganic compounds—novel compositions of matter within known structure types, or even compounds with completely new crystal structures—constitutes an important goal of solid-state and materials chemistry. Some fractions of new compounds can eventually lead to new structural and functional materials that enhance the efficiency of existing technologies or even enable completely new technologies. Materials researchers eagerly welcome new approaches to the discovery of new compounds, especially those that offer the promise of accelerated success. The recent report from a group of scientists at Google who employ a combination of existing data sets, high-throughput density functional theory calculations of structural stability, and the tools of artificial intelligence and machine learning (AI/ML) to propose new compounds is an exciting advance. We examine the claims of this work here, unfortunately finding scant evidence for compounds that fulfill the trifecta of novelty, credibility, and utility. While the methods adopted in this work appear to hold promise, there is clearly a great need to incorporate domain expertise in materials synthesis and crystallography.



From micro to macro adds layers of modeling complexity



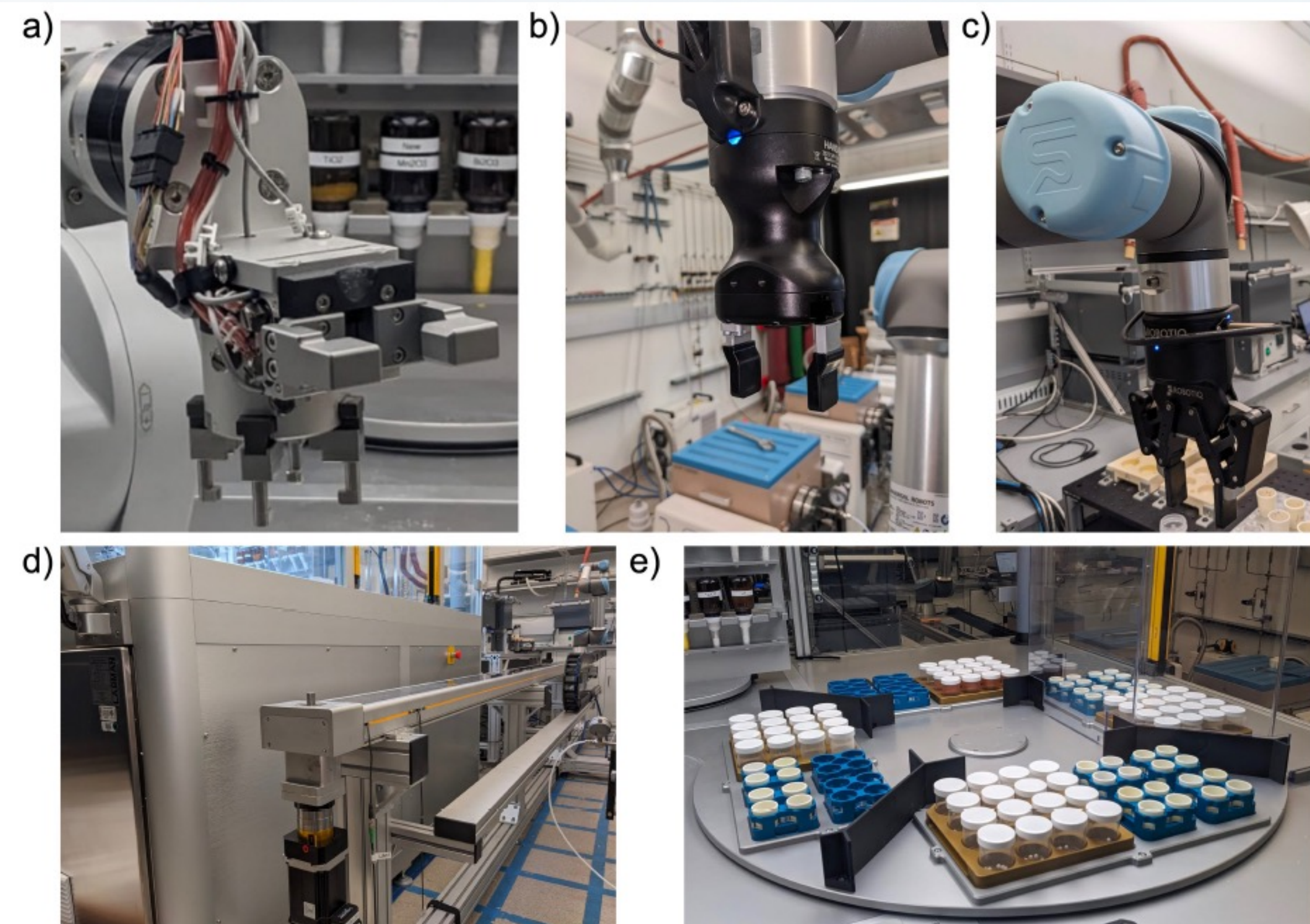
Source: "Opportunities and challenges in understanding complex functional materials" Nature Communications 1 October 2019

High throughput / rapid experimentation is also challenging



A-Lab, a facility at Berkeley Lab where artificial intelligence guides robots in making new materials.

Photo credit: Marilyn Sargent/Berkeley Lab



Extended Data Fig. 2 | Robotic installations for sample transfer in the A-Lab. Grippers on the UR5e robotic arms that are used for sample preparation (a), loading/unloading of crucible racks to/from the box furnaces (b) and sample retrieval and characterization (c). d, Linear rail used to increase the working

envelope of the robotic arm that loads/unloads crucible racks to/from the furnaces. e, Carousel used to organize and move samples in the sample preparation station.

Source: "An autonomous laboratory for the accelerated synthesis of novel materials", Nature Vol 624 December 7 2023

The first US startup in AI+ materials was founded in 2013

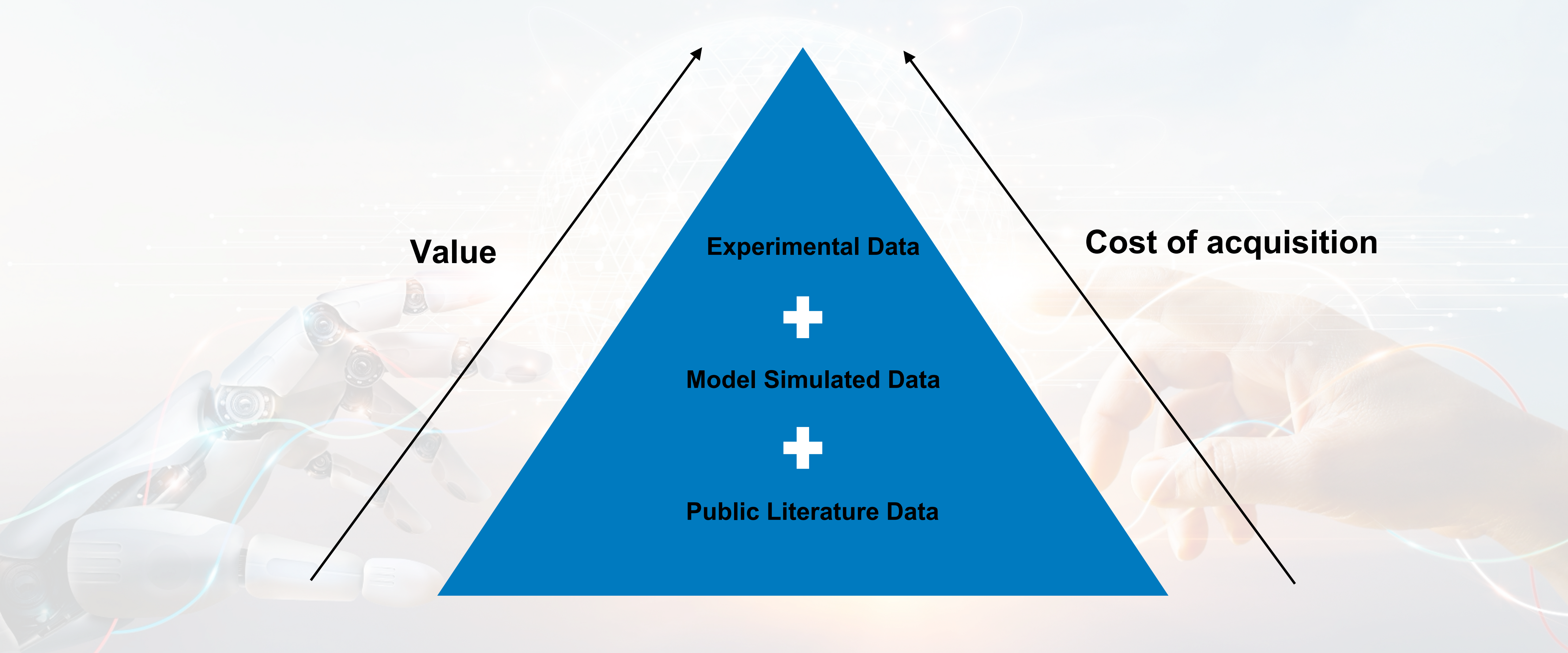
CITRINE 
INFORMATICS

Founded 2013

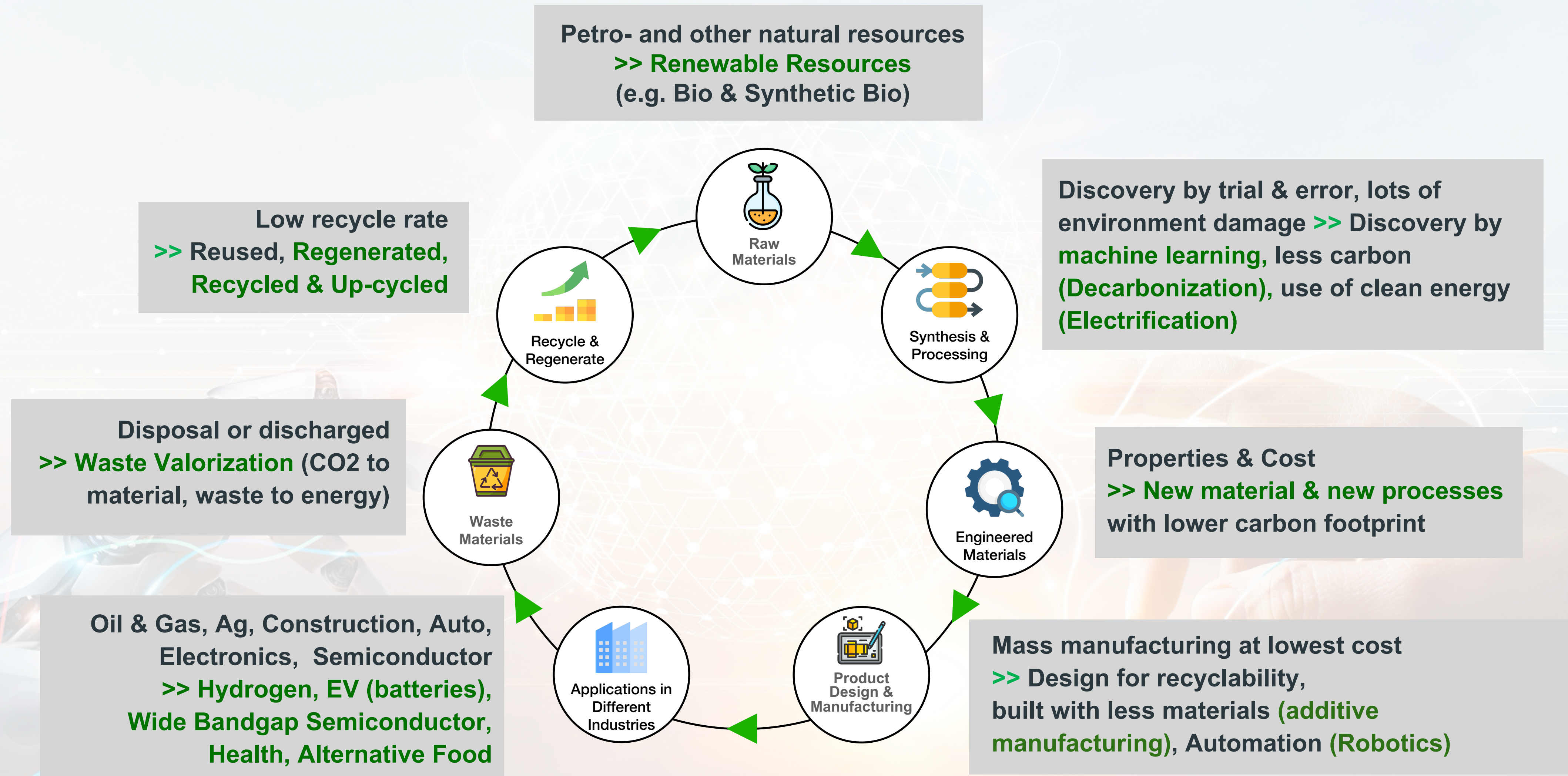


High quality data remains the #1 challenge

- The most valuable is also the most costly



2nd biggest challenge – finding good application in a long value chain



Currently more platform companies than product companies in AI+Materials

Overseas

Vertical field



Platform

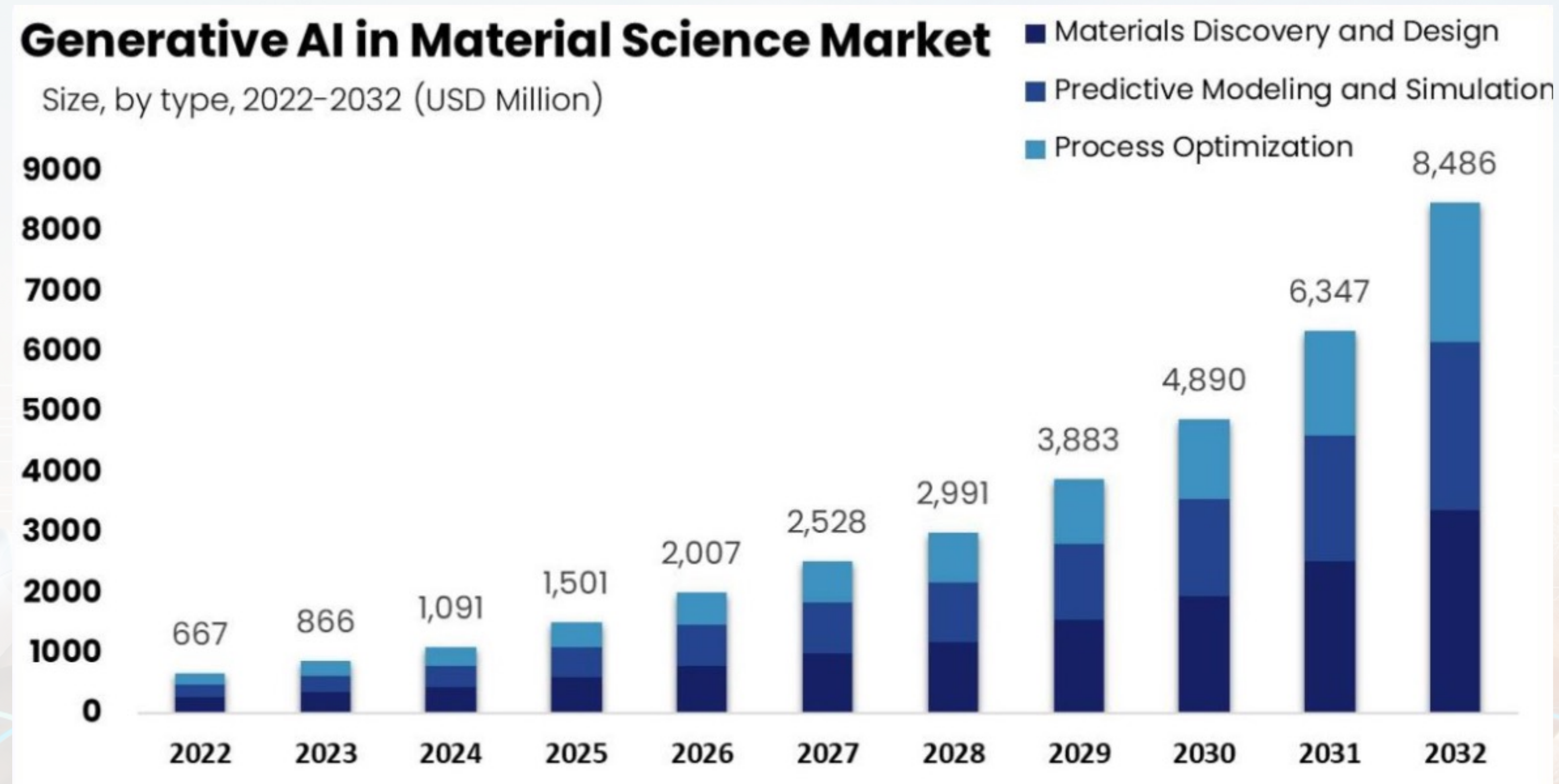
Products



Vertical field

Domestic

AI + Materials is expected to grow at CAGR of ~30% to \$ 8.5 B USD by 2032



Source: MarketResearch.biz report "Generative AI in Material Science"