Materials Informatics

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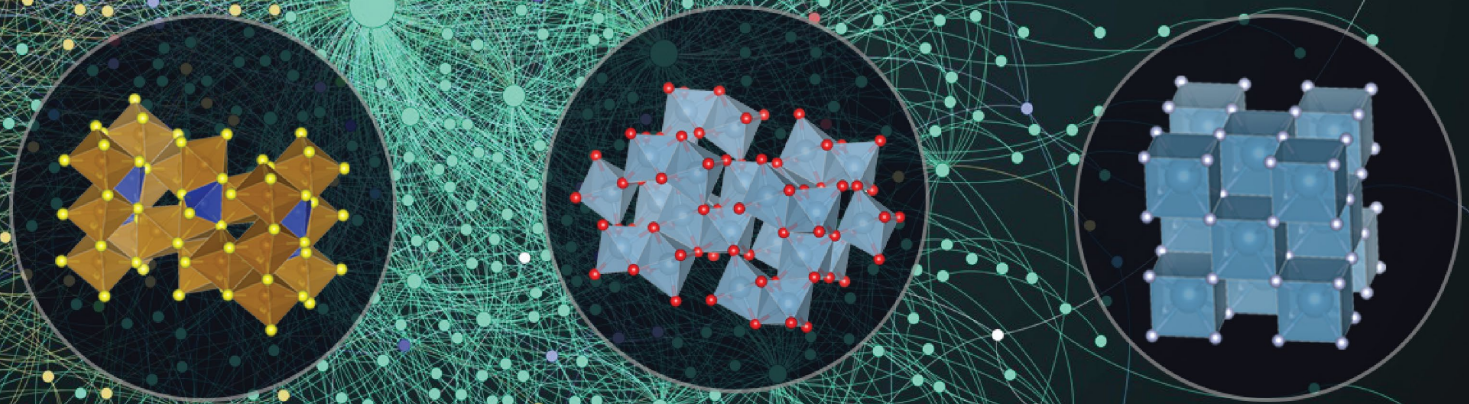
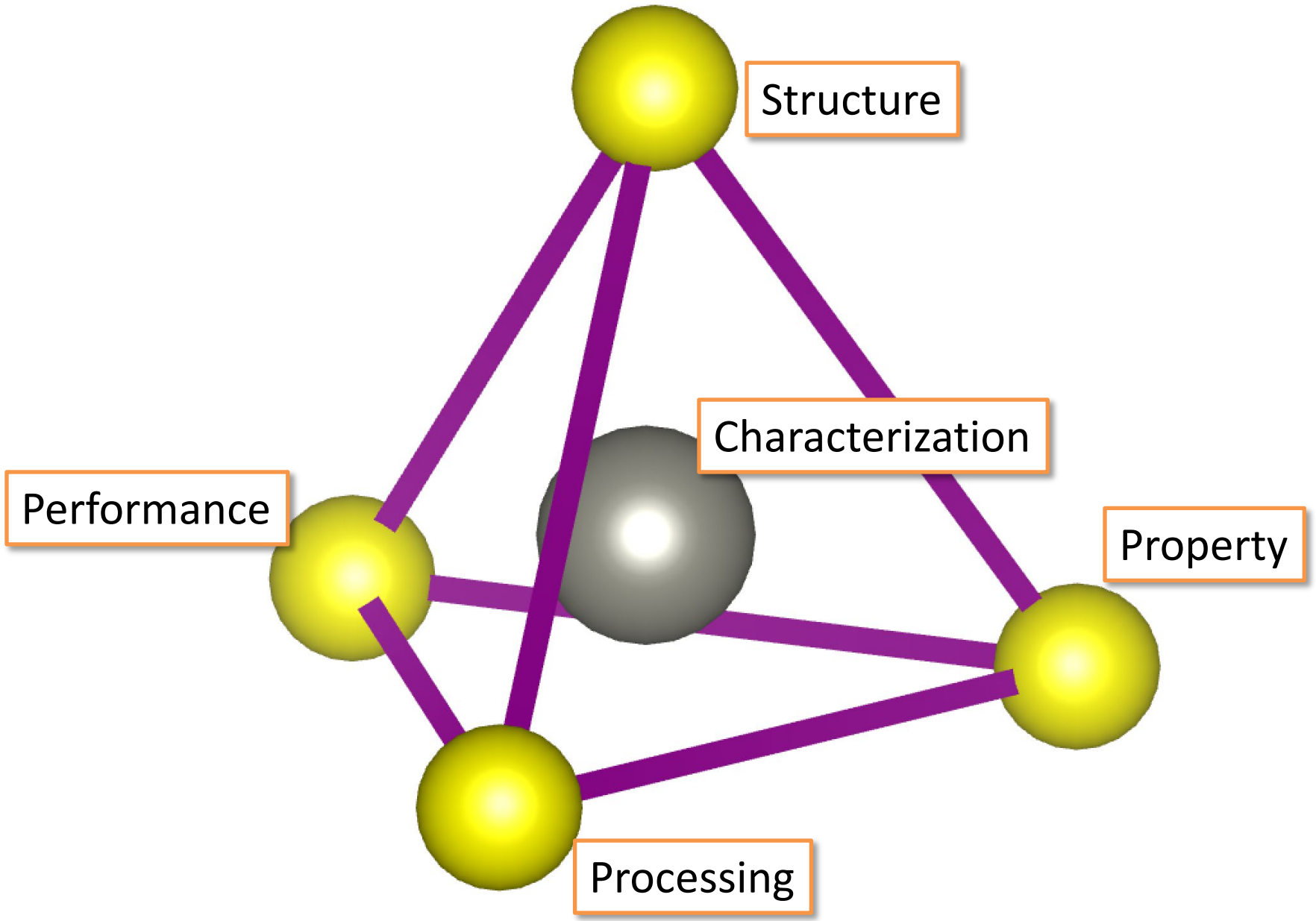
What is Materials Informatics?



Materials Informatics is data science applied to materials science



Materials Informatics is data science applied to materials science

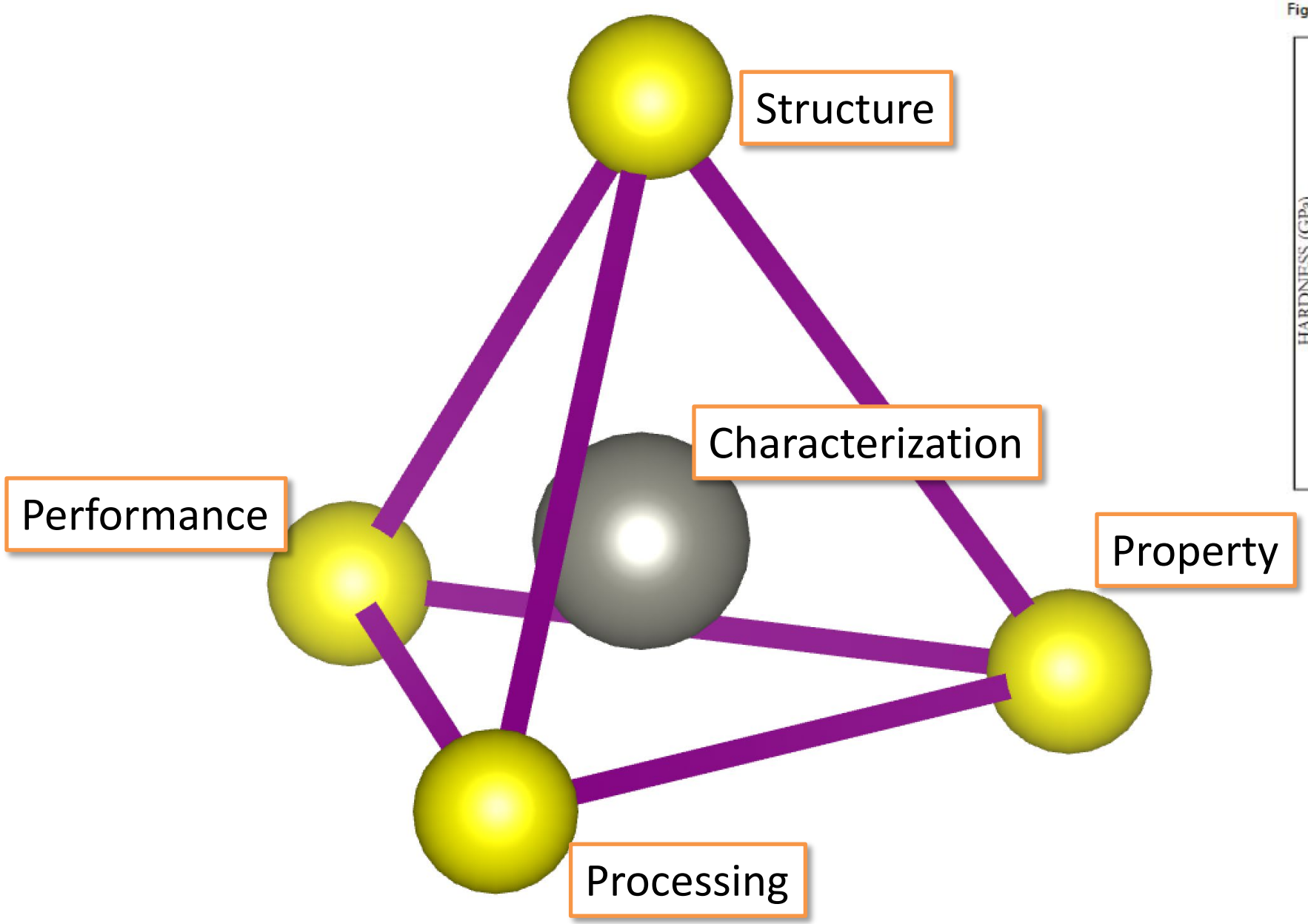
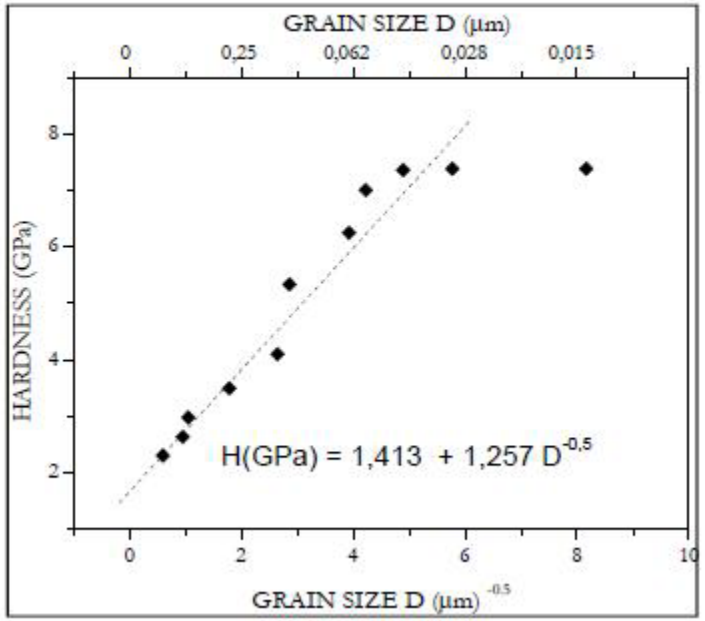


Figure 3. Hall-Petch ratio for 0.6%C steel

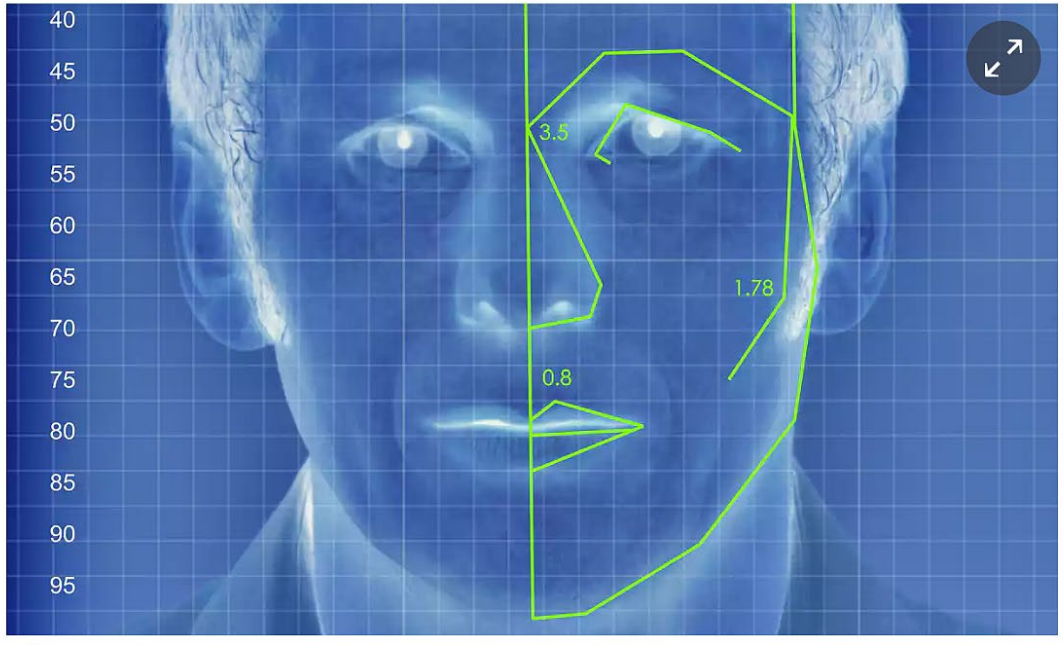


ML can extract highly complex trends in data!

theguardian

New AI can guess whether you're gay or straight from a photograph

An algorithm deduced the sexuality of people on a dating site with up to 91% accuracy, raising tricky ethical questions



An illustrated depiction of facial analysis technology similar to that used in the experiment. Illustration: Alamy

Most popular in US


Trump at UN: US may 'have no choice but to totally destroy North Korea' - live


Hurricane Maria: Storm grows in force to category 5 as Caribbean battered again - live


Where is Hurricane Maria heading? Mapping the path of destruction

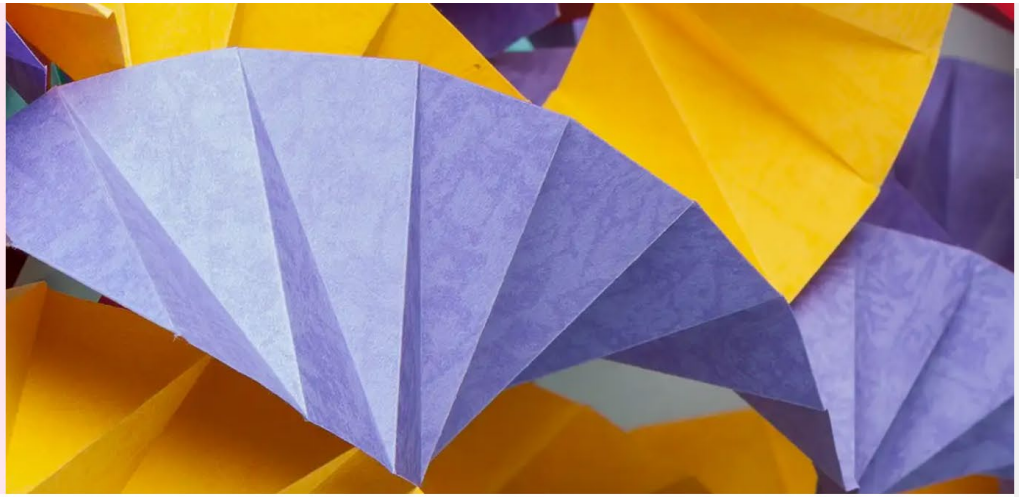

Russian helicopter

ML has already made incredible advances in science

BLOG POST
RESEARCH

30 NOV 2020

AlphaFold: a solution to a 50-year-old grand challenge in biology



SHARE

AUTHORS

TAt The AlphaFold team

Proteins are essential to life, supporting practically all its functions. They are large complex molecules, made up of chains of amino acids, and what a protein does largely depends on its unique 3D structure. Figuring out what shapes proteins fold into is known as the "protein folding problem", and has stood as a grand challenge in biology for the past 50 years. In a major scientific advance, the latest version of our AI system AlphaFold has been recognised as a solution to this grand challenge by the organisers of the biennial Critical Assessment of protein Structure Prediction (CASP). This breakthrough demonstrates the impact AI can have on scientific discovery and its potential to dramatically accelerate progress in some of the most fundamental fields that explain and shape our world.

A protein's shape is closely linked with its function, and the ability to predict this structure unlocks a greater understanding of what it does and how it works. Many of the world's greatest challenges, like developing treatments for diseases or finding enzymes that break down industrial waste, are fundamentally tied to proteins and the role they play.

BACK TO TOP

ML has already made incredible advances in science

CASE STUDY

CITRINE INFORMATICS

citrine.io • info@citrine.io

CITRINE ACCELERATES DEVELOPMENT TIME FOR ADDITIVE MANUFACTURING

3D PRINTABLE AEROSPACE-GRADE ALLOY DEVELOPMENT REDUCED FROM YEARS TO DAYS

CITRINE INFORMATICS HRL LABORATORIES

Aluminum 7A77.60L powder from HRL. Copyright 2019 HRL Laboratories, LLC.

Al 7A77
New alloy!

EXECUTIVE SUMMARY

FAST TIME TO MARKET
TWO YEARS AFTER RESEARCH PUBLICATION - COMMERCIALIZED WITH NASA AS THE FIRST CUSTOMER

TIME SAVED
EXPERIMENTAL LAB WORK REDUCED FROM YEARS TO DAYS DUE TO MATERIALS INFORMATICS APPROACH

PERFORMANCE IMPROVED
NEW ALLOY POWDER RETAINS STRENGTH WHEN USED IN OFF-THE-SHELF 3D PRINTING EQUIPMENT

FIRST TO MARKET
FIRST ADDITIVE ALLOY REGISTERED BY THE ALUMINUM ASSOCIATION

Materials Informatics is only a few decades old

materialstoday
Volume 8, Issue 10, October 2005, Pages 38-45

Review Feature

Materials informatics

Krishna Rajan ✉

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https://doi.org/10.1016/S1369-7021(05)71123-8

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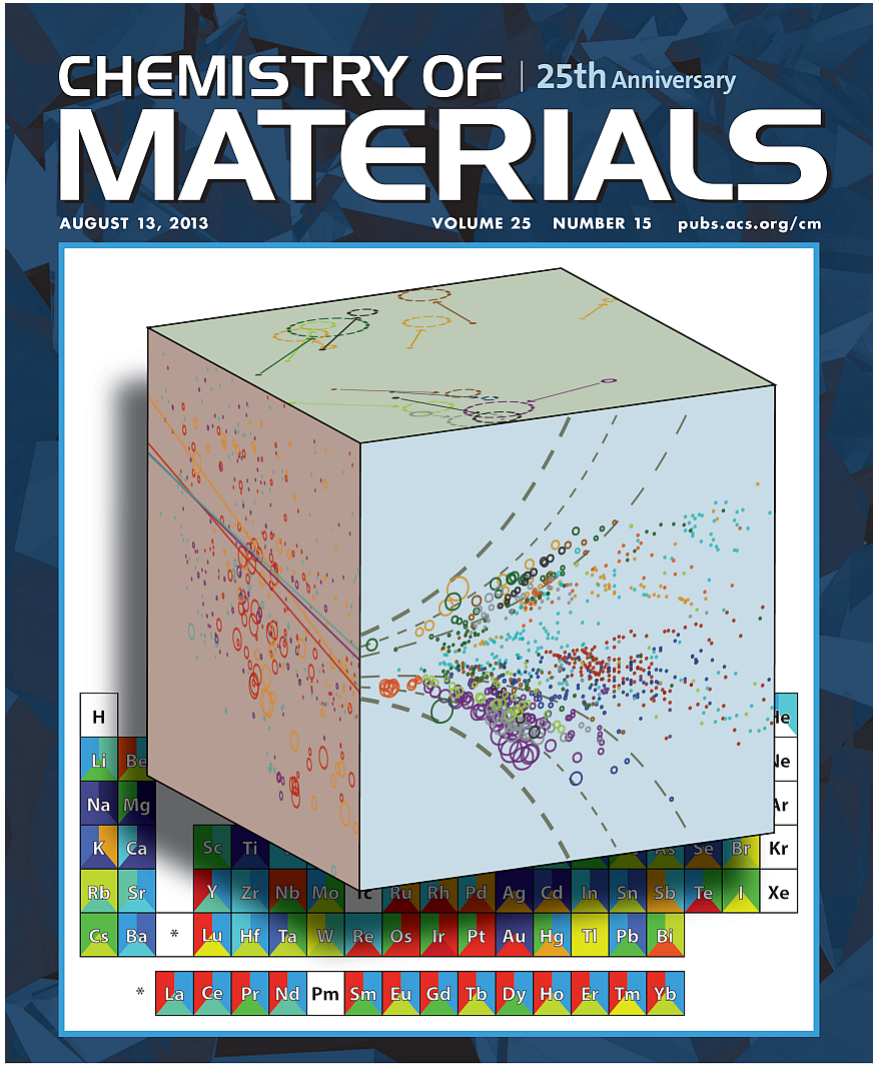
Seeking structure-property relationships is an accepted paradigm in materials science, yet these relationships are often not linear, and the challenge is to seek patterns among multiple lengthscales and timescales. There is rarely a single multiscale theory or experiment that can meaningfully and accurately capture such information. In this article, we outline a process termed 'materials informatics' that allows one to survey complex, multiscale information in a high-throughput, statistically robust, and yet physically meaningful manner. The application of such an approach is shown to have significant impact in materials design and discovery.

Previous article in issue Next article in issue

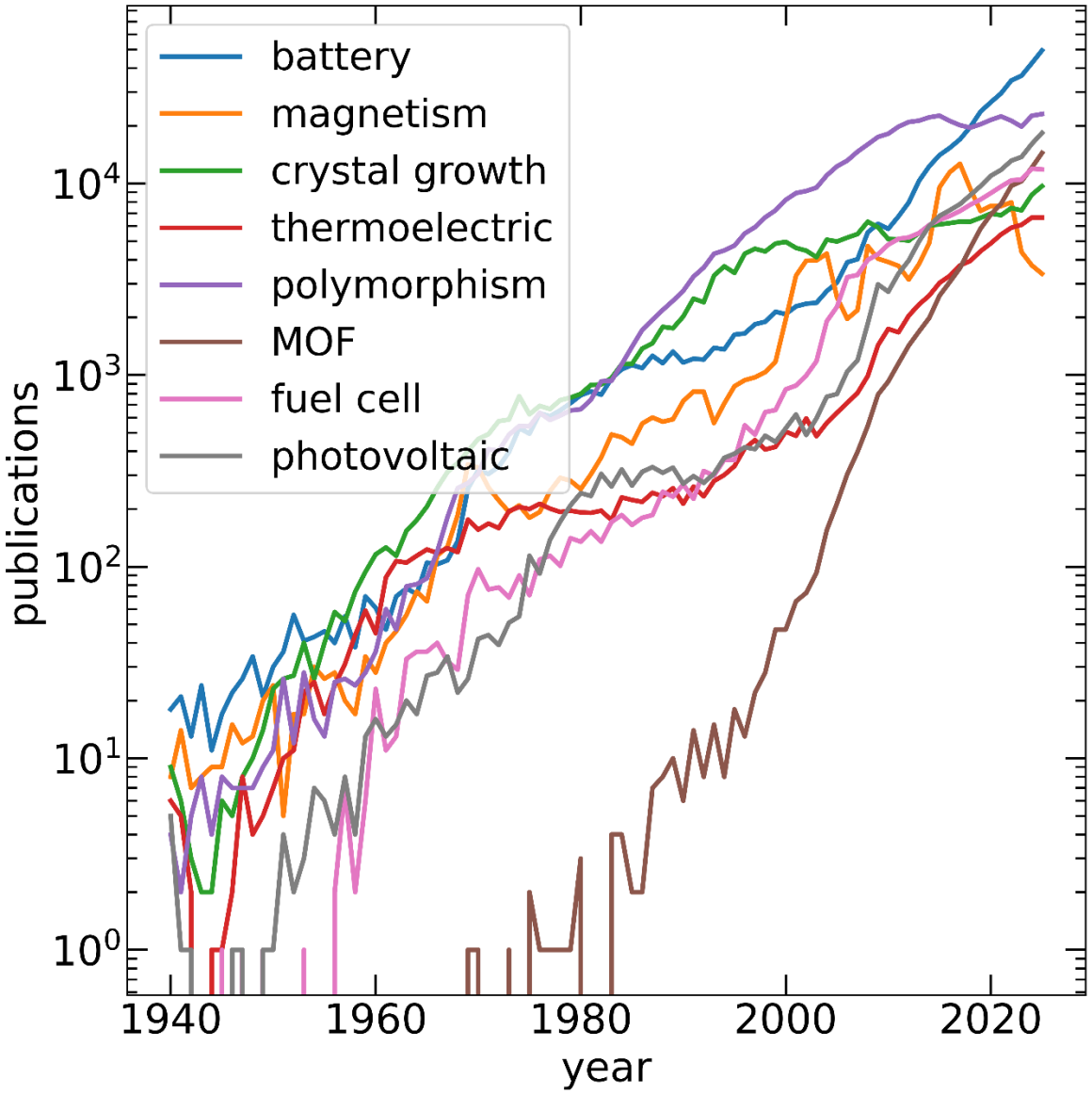
In the early days… nobody knew what they were doing

We initially used “big data” to write analytical reviews

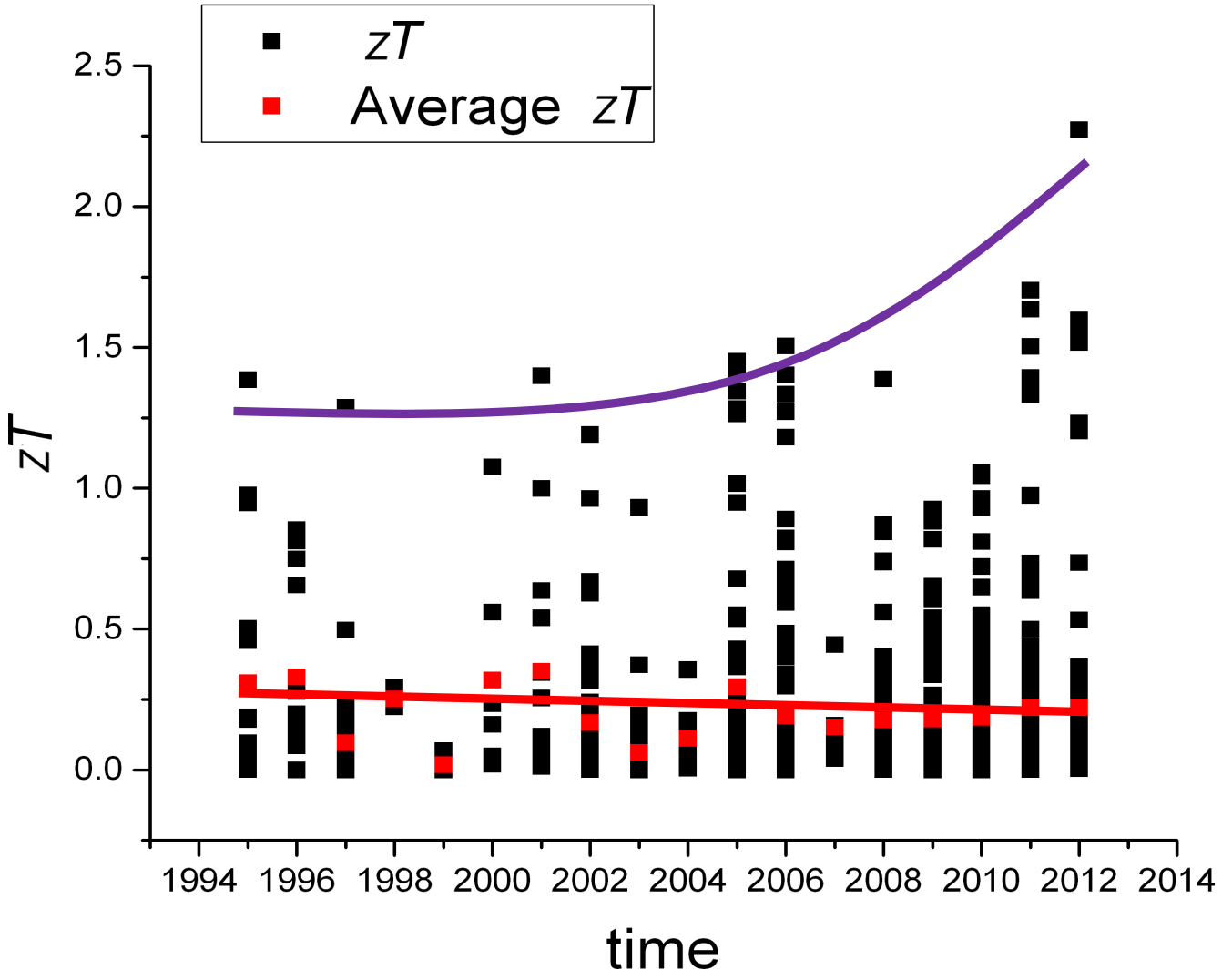


Sparks et al. (2016) *Script. Mat.*
Gaultois et al. (2013) *Chem Mat.*
Ghadbeigi et al. (2016) *Energy Environ. Sci.*
Gaultois et al. (2016) *APL Mat.*

Why do we need data-driven materials science?

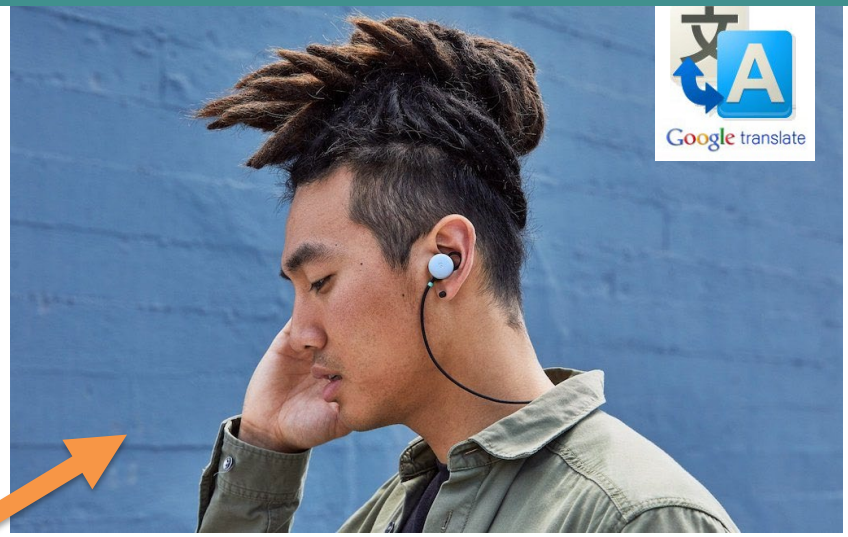


Most materials improvements are incremental



Breakthroughs are the uncommon exception

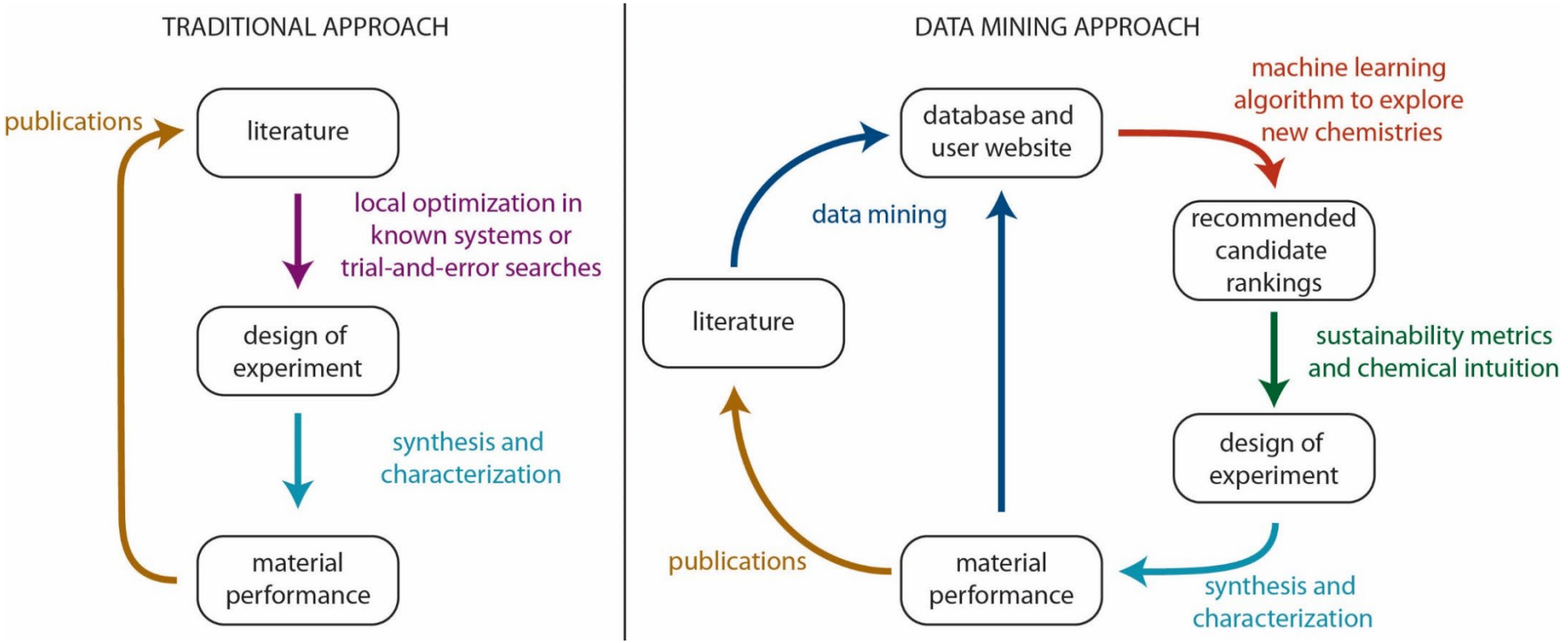
Useful relationships can be learned from data directly!



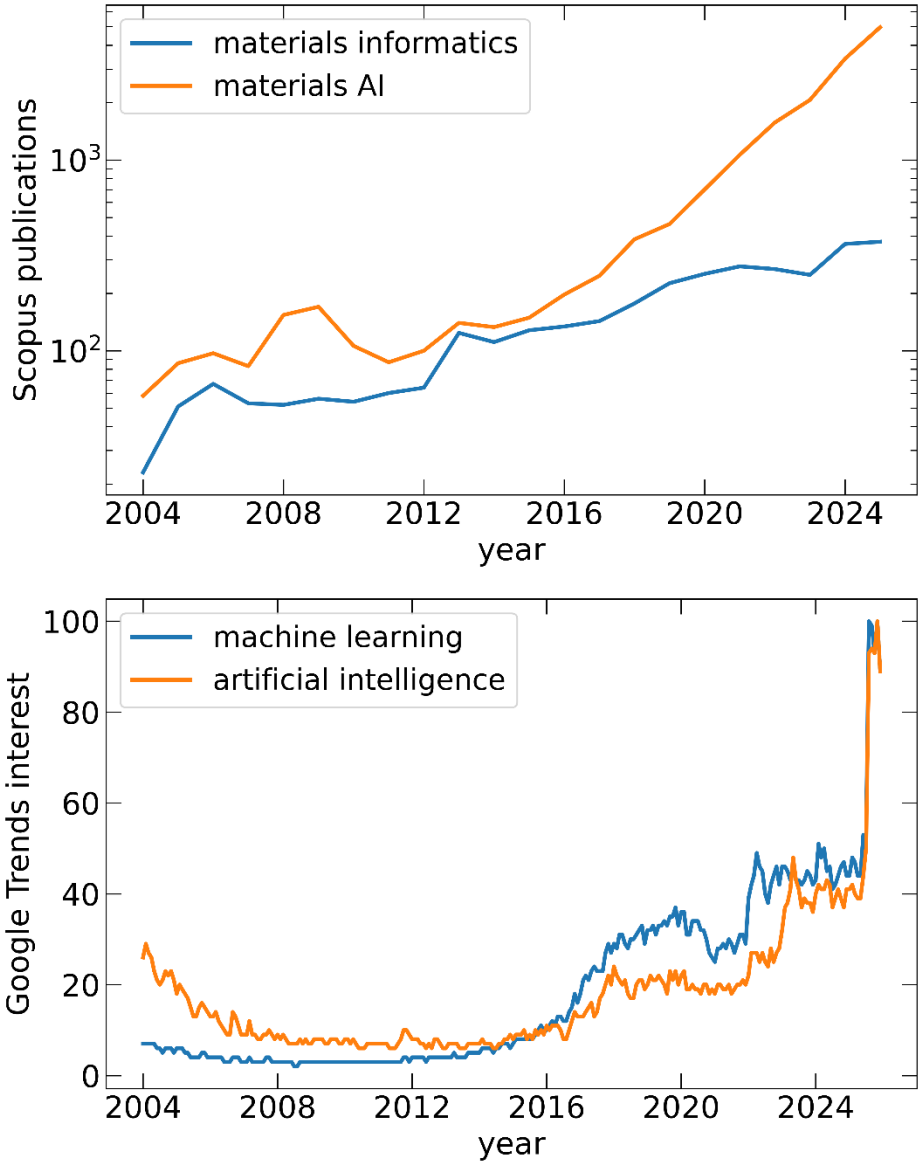
Are there "materials genes" responsible for desired behavior?

- Equip the next generation workforce
- Enable a paradigm shift in materials development
- Integrate experiments, computation, and theory
- Facilitate access to materials data

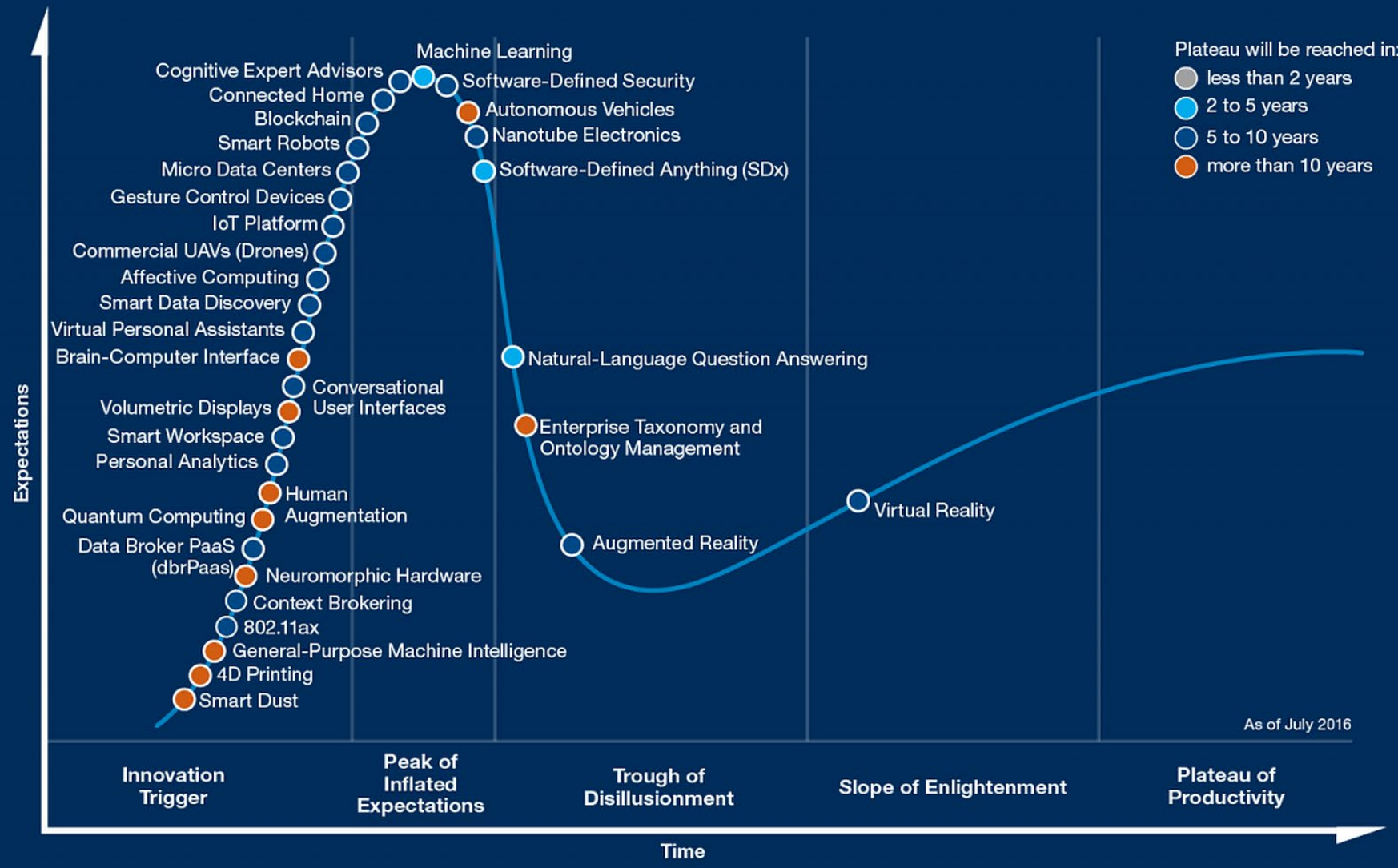
New tools of discovery are needed for “chemical whitespace”



Is materials informatics a passing fad, or here to stay?



Gartner Hype Cycle for Emerging Technologies, 2016



Source: Gartner

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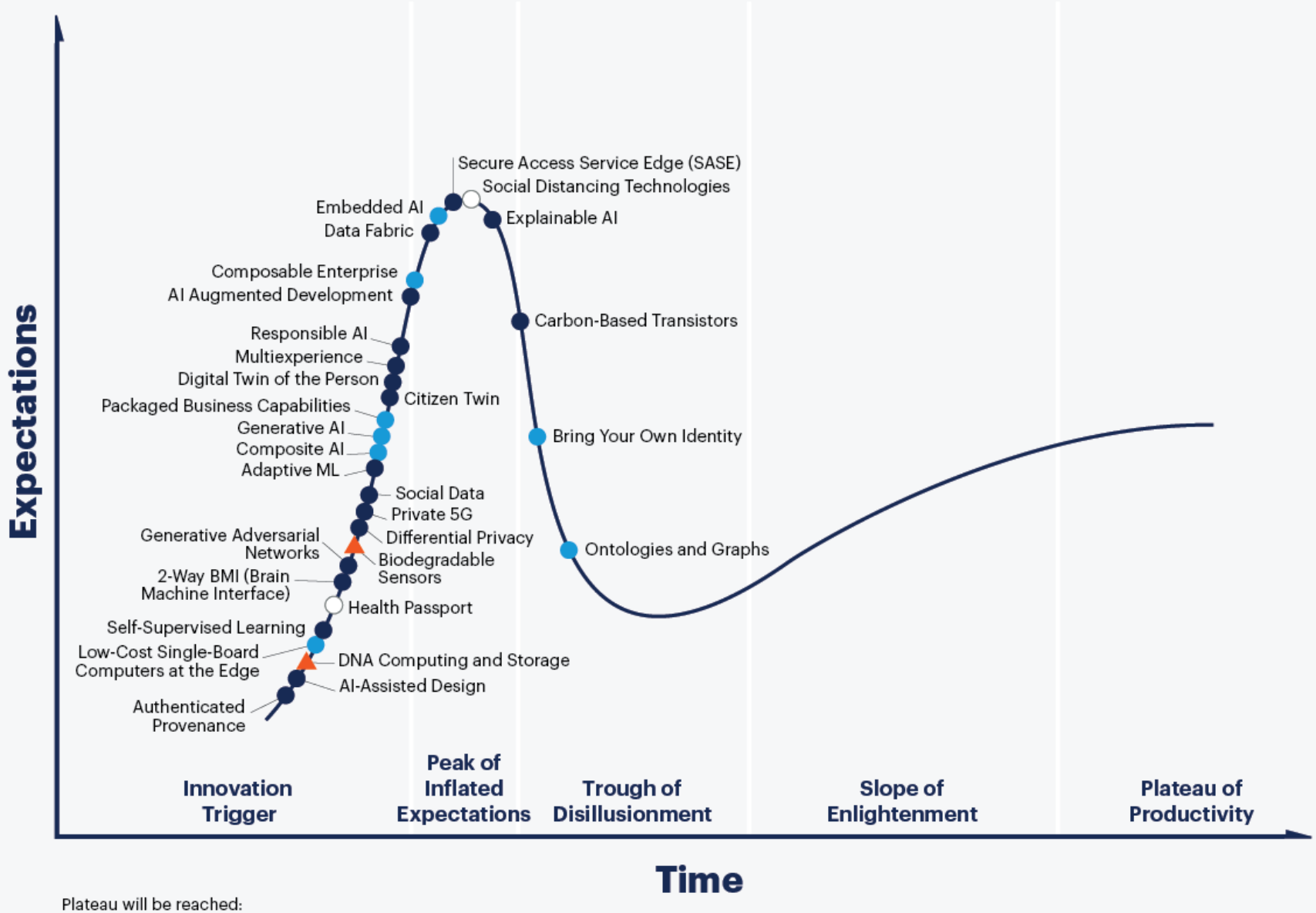
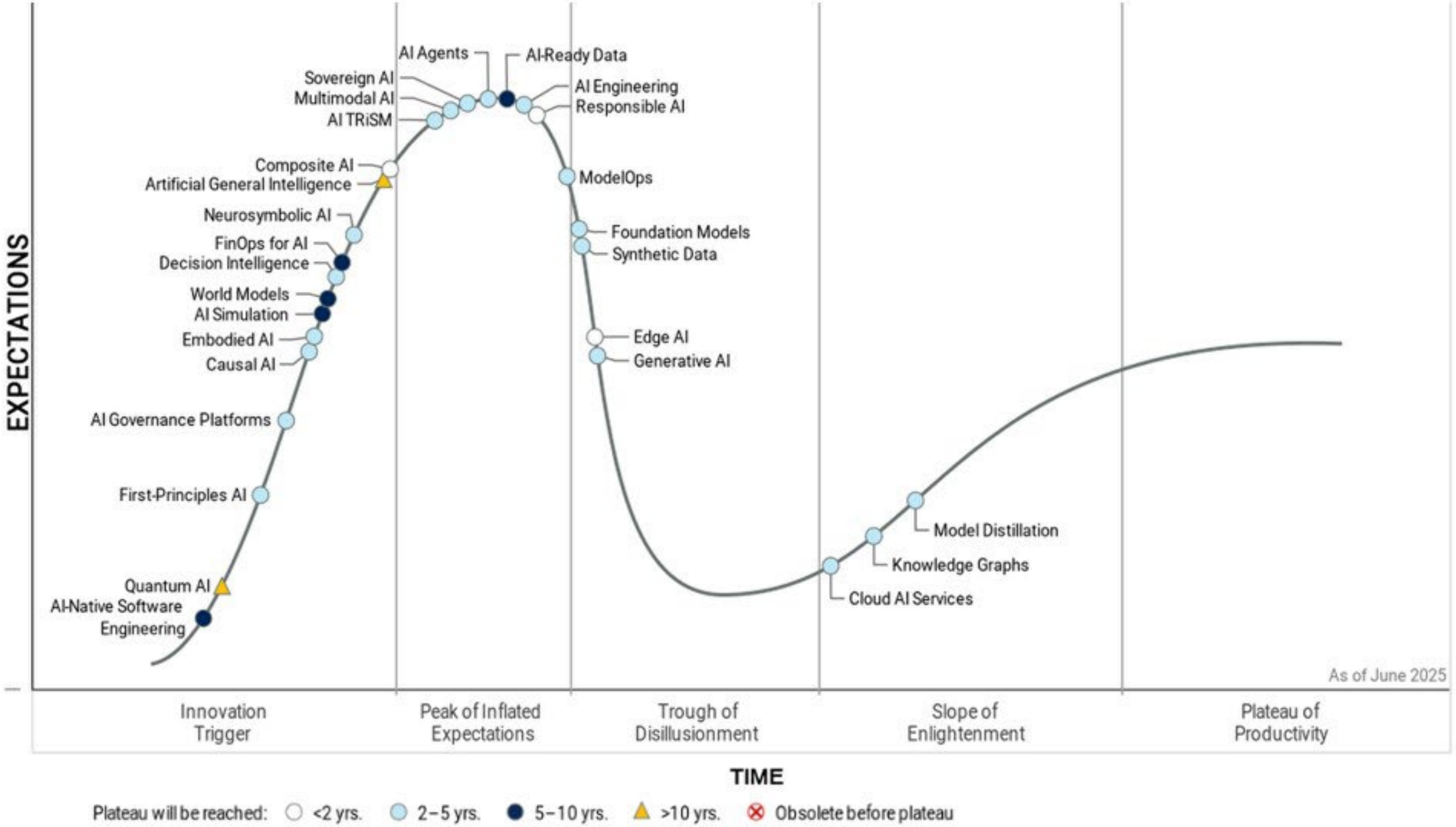
Gartner

Hype Cycle for Emerging Technologies, 2020




EXPECTATIONS
AI Agents
AI-Ready Data
Sovereign AI
Multimodal AI
AI TRiSM
AI Engineering
Responsible AI
Composite AI
Artificial General Intelligence
ModelOps
Neurosymbolic AI
FinOps for AI
Decision Intelligence
Foundation Models
Synthetic Data
World Models
AI Simulation
Embodied AI
Causal AI
Edge AI
Generative AI
AI Governance Platforms
First-Principles AI
Model Distillation
Knowledge Graphs
Cloud AI Services
Quantum AI
AI-Native Software Engineering
As of June 2025
Innovation Trigger
Peak of Inflated Expectations
Trough of Disillusionment
Slope of Enlightenment
Plateau of Productivity
TIME
Plateau will be reached:
<2 yrs.
2–5 yrs.
5–10 yrs.
>10 yrs.
Obsolete before plateau

Gartner

How are materials discovered?