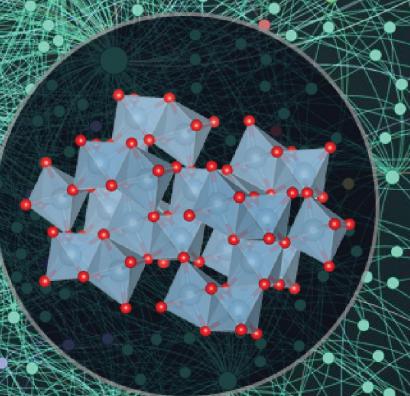
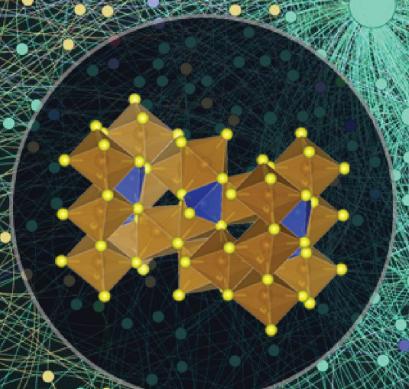


Materials Informatics

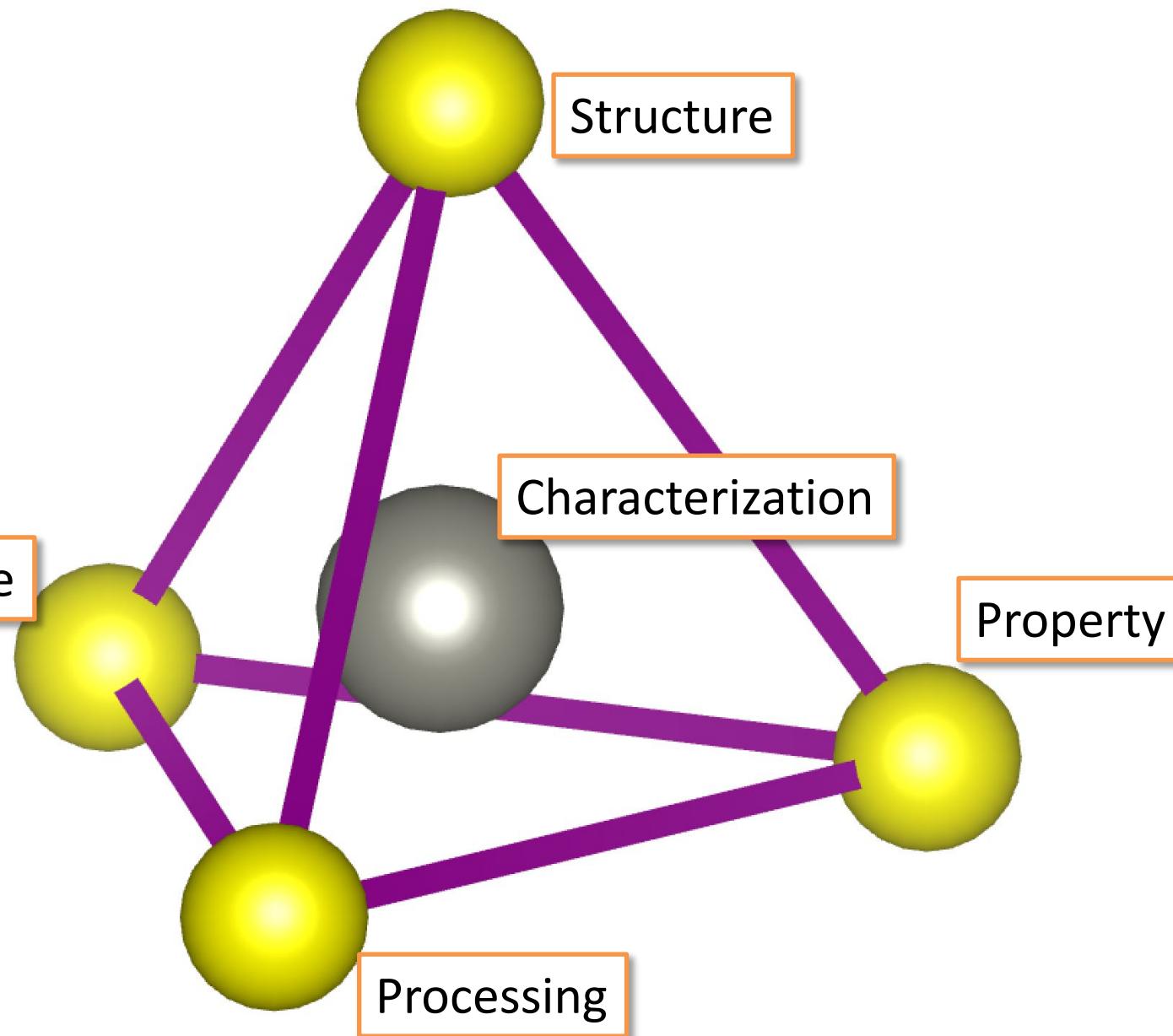


Taylor D. Sparks
University of Utah, Materials Science and Engineering Department

What is Materials Informatics?



Materials Informatics is data science applied to materials science



Materials Informatics is data science applied to materials science

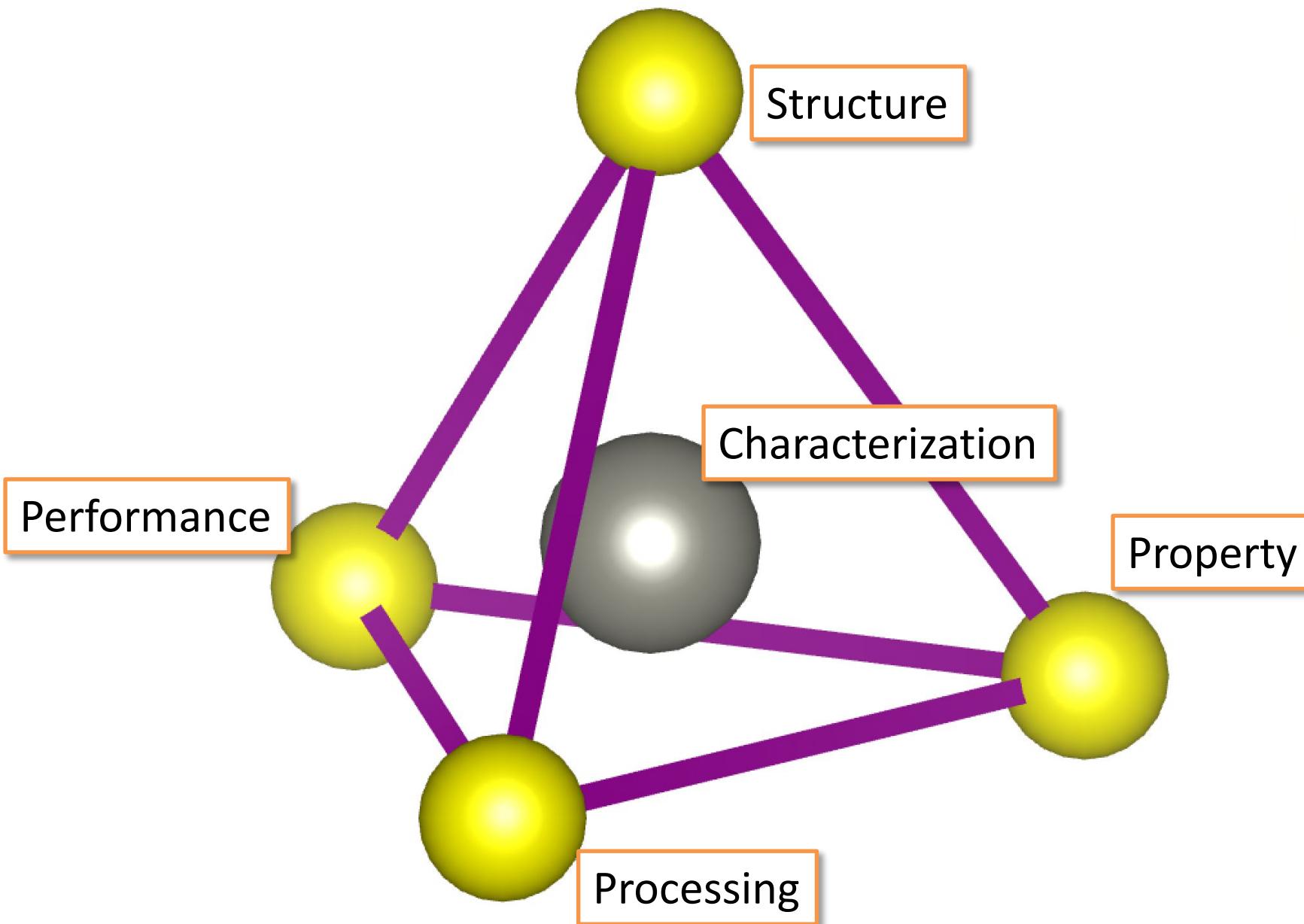
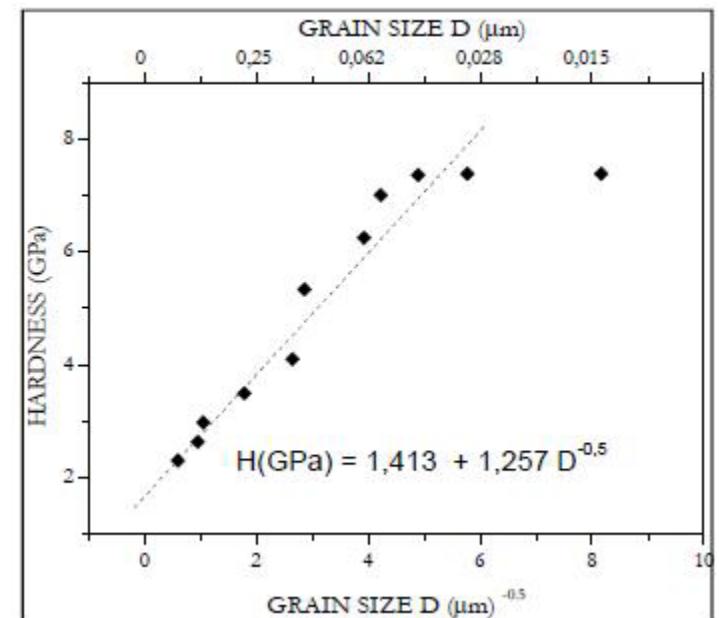


Figure 3. Hall-Petch ratio for 0.6%C steel



Machine learning is capable of extracting highly complex trends from data

The screenshot shows a news article from theguardian.com. The header features the site's logo in white on a dark blue background. Below the logo is a navigation bar with links to various sections: world, opinion, sports, soccer, tech, arts, lifestyle, fashion, business, travel, environment, and an 'all sections' button. The main headline reads: "New AI can guess whether you're gay or straight from a photograph". A subtext below the headline states: "An algorithm deduced the sexuality of people on a dating site with up to 91% accuracy, raising tricky ethical questions". To the left of the text is a graphic illustration of a face with a grid overlay, showing green outlines and numerical values (3.5, 0.8, 1.78) representing facial analysis data. On the right side of the article, there is a sidebar titled "Most popular in US" featuring three news items with images and titles: "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", and "Where is Hurricane Maria heading? Mapping the path of destruction". At the bottom of the page, a footer note says: "An illustrated depiction of facial analysis technology similar to that used in the experiment. Illustration: Alamy".

the guardian

world opinion sports soccer tech arts lifestyle fashion business travel environment ≡ all sections

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

A close-up illustration of a person's face with a grid overlay. Green lines and numbers (3.5, 0.8, 1.78) highlight specific facial features, representing the data points used by the AI algorithm.

Most popular in US

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

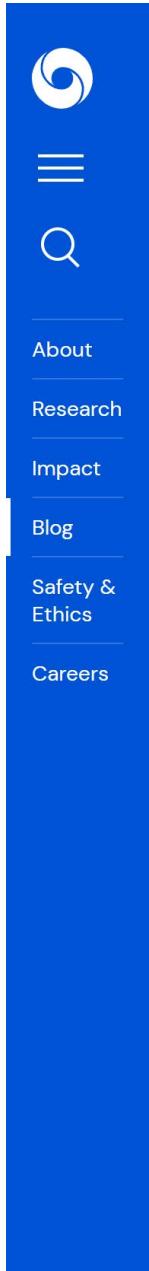
 Hurricane Maria: Storm grows in force to category 5 as Caribbean battered again - live

 Where is Hurricane Maria heading? Mapping the path of destruction

 Russian helicopter

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

Machine learning has already made huge impacts on science and engineering!



30 NOV 2020

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

SHARE



AUTHORS



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 An upward-pointing blue arrow icon.

Machine learning has already made huge impacts on science and engineering!



CITRINE ACCELERATES DEVELOPMENT TIME FOR ADDITIVE MANUFACTURING

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



AI 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!



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



Review Feature

Materials informatics

Krishna Rajan

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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 of materials informatics, nobody knew what they were doing



Dan Ariely

January 6, 2013 ·

Big data is like teenage sex: everyone talks about it, nobody really knows how to do it, everyone thinks everyone else is doing it, so everyone claims they are doing it...

13

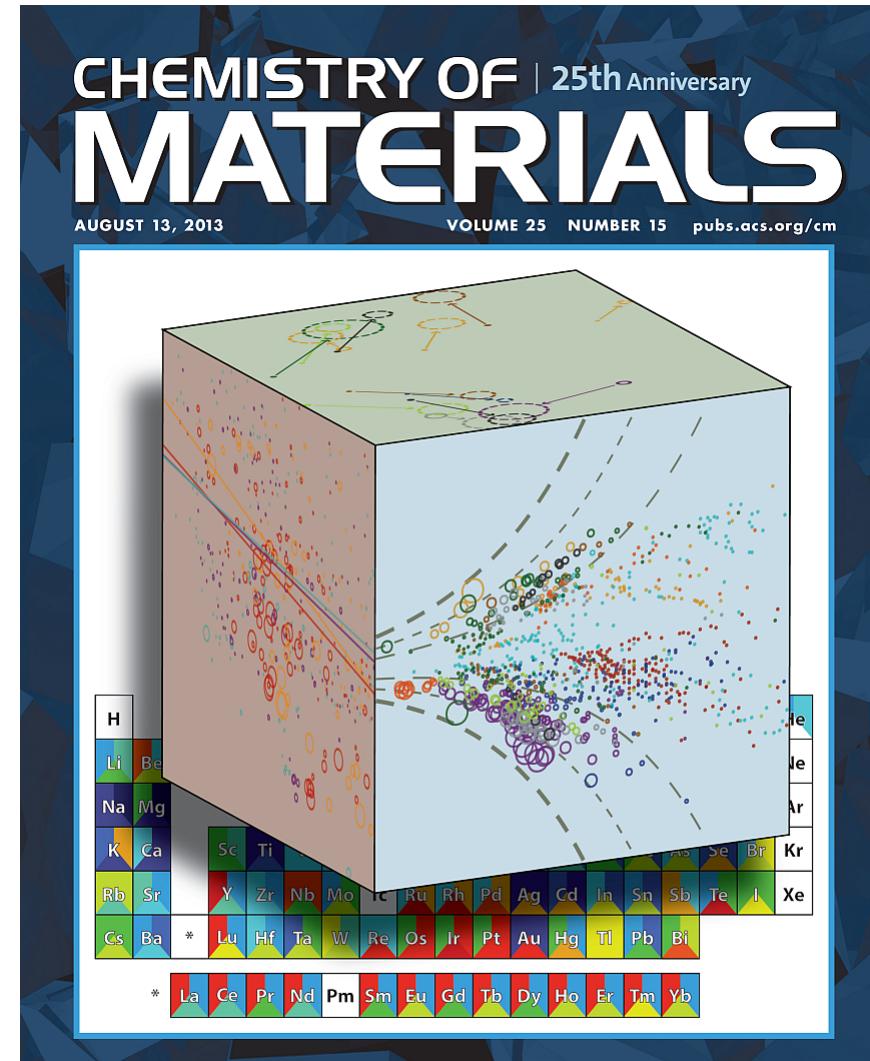
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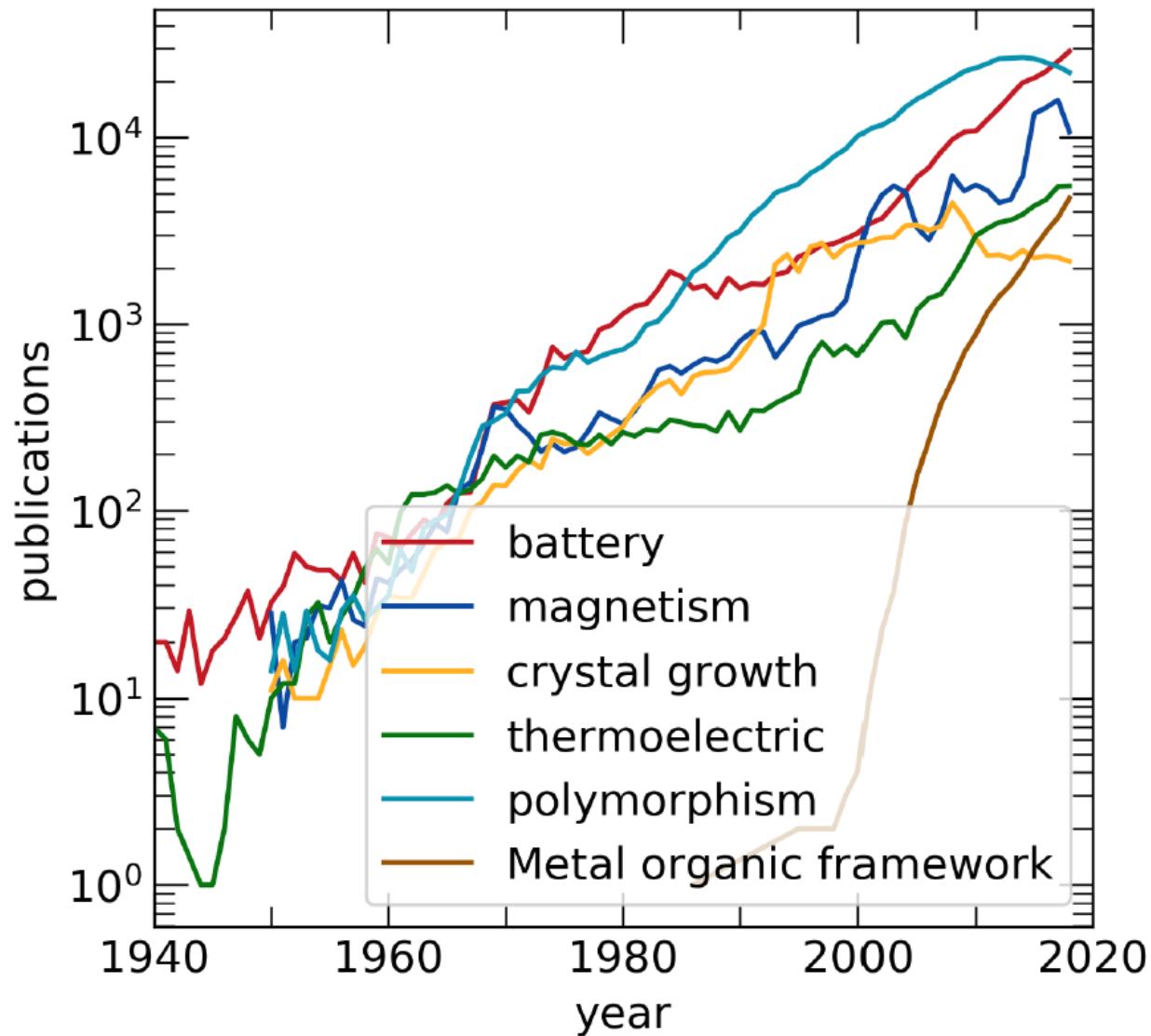
We initially only used “big data” to write analytical reviews



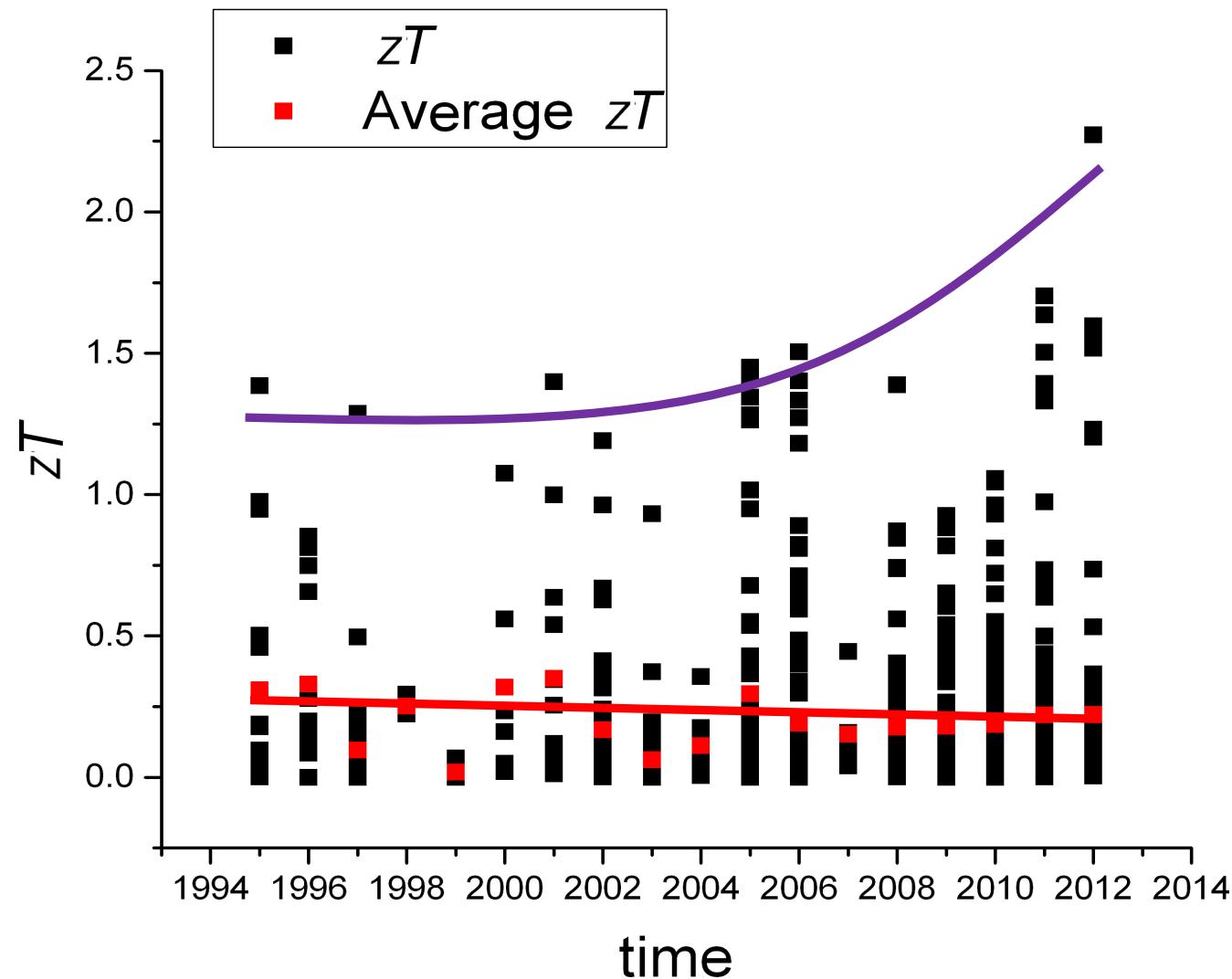
- Sparks et al. (2016) *Script. Mat.*
Gaultois et al. (2013) *Chem Mat.*
Ghadbeigi et al. (2016) *Energy Environ. Sci.*
Gaultois et al. (2016) *APL Mat.*



Why do we need data-driven materials science?



Most materials research is incremental, breakthroughs are the exception!



Useful information can be mined from large datasets without domain knowledge!

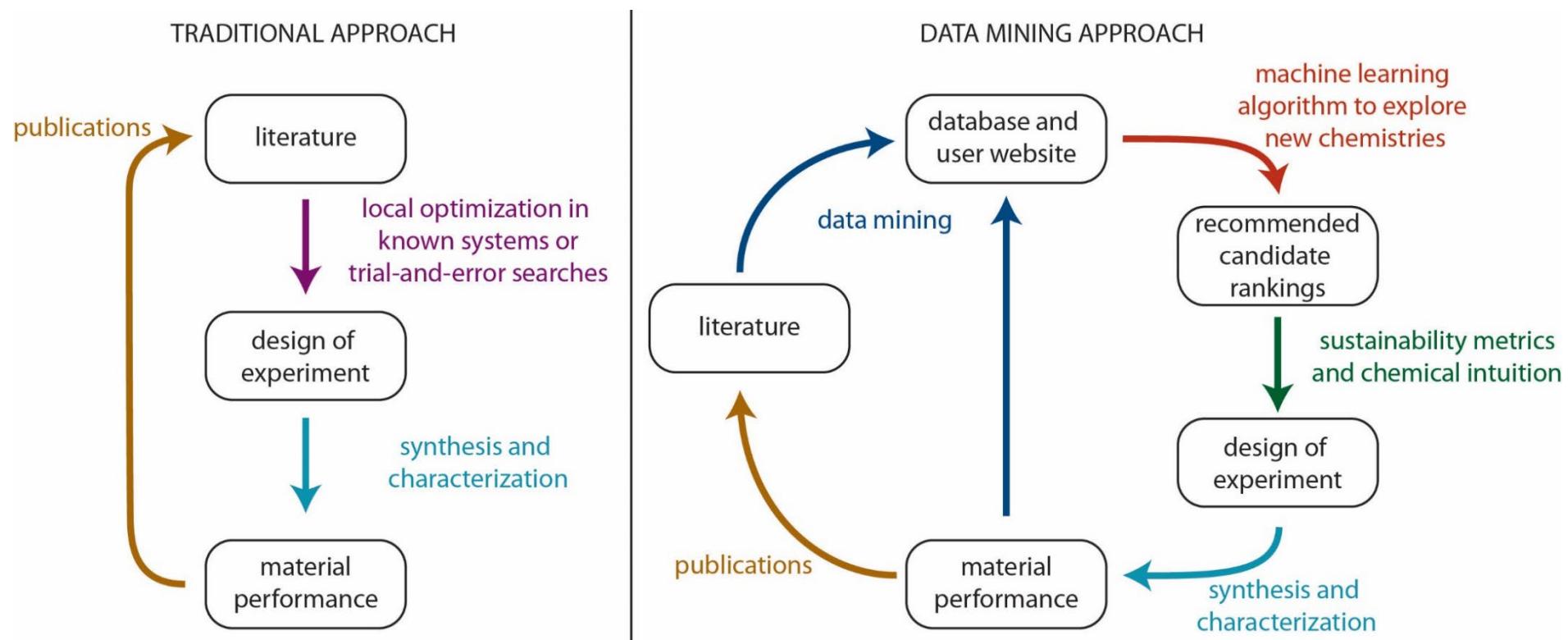


Are there materials “genes” responsible for their properties and performance?

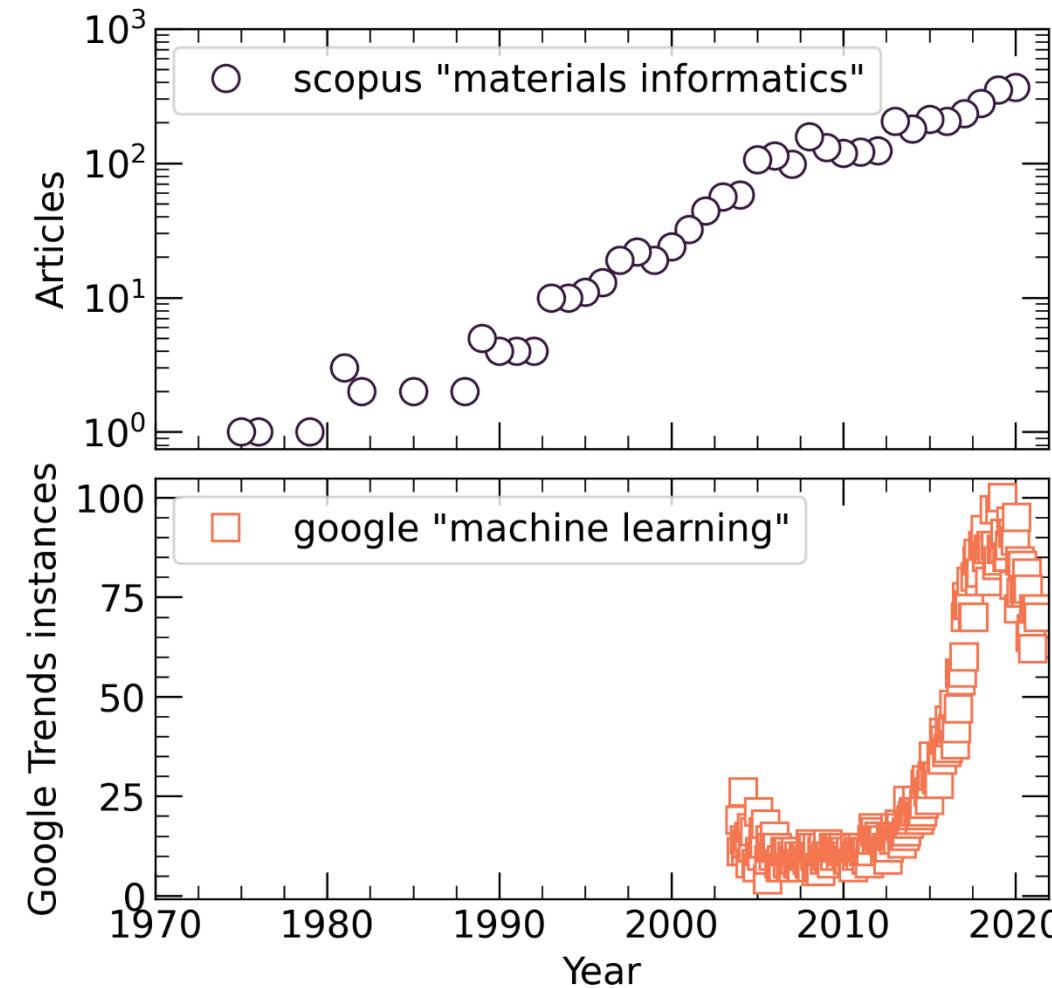


- Equip the next generation workforce
- Enable a paradigm shift in materials development
- Integrate experiments, computation, and theory
- Facilitate access to materials data

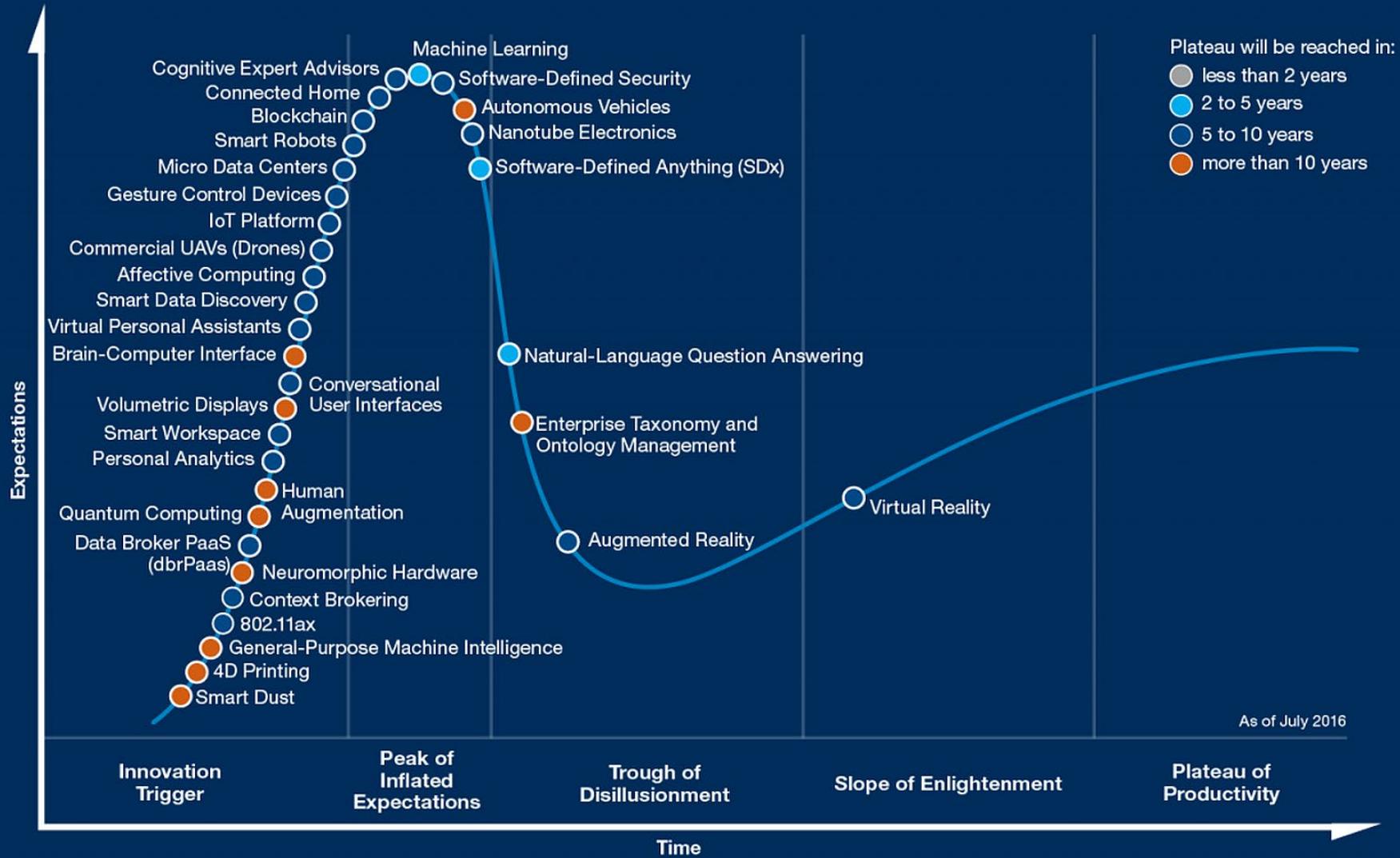
New tools of discovery are needed to explore chemical whitespace



Is materials informatics a passing fad or here to stay?



Gartner Hype Cycle for Emerging Technologies, 2016



Hype Cycle for Emerging Technologies, 2020



Plateau will be reached:

○ less than 2 years

● 2 to 5 years

● 5 to 10 years

▲ more than 10 years

✗ obsolete before plateau

As of July 2020

How are materials discovered?

