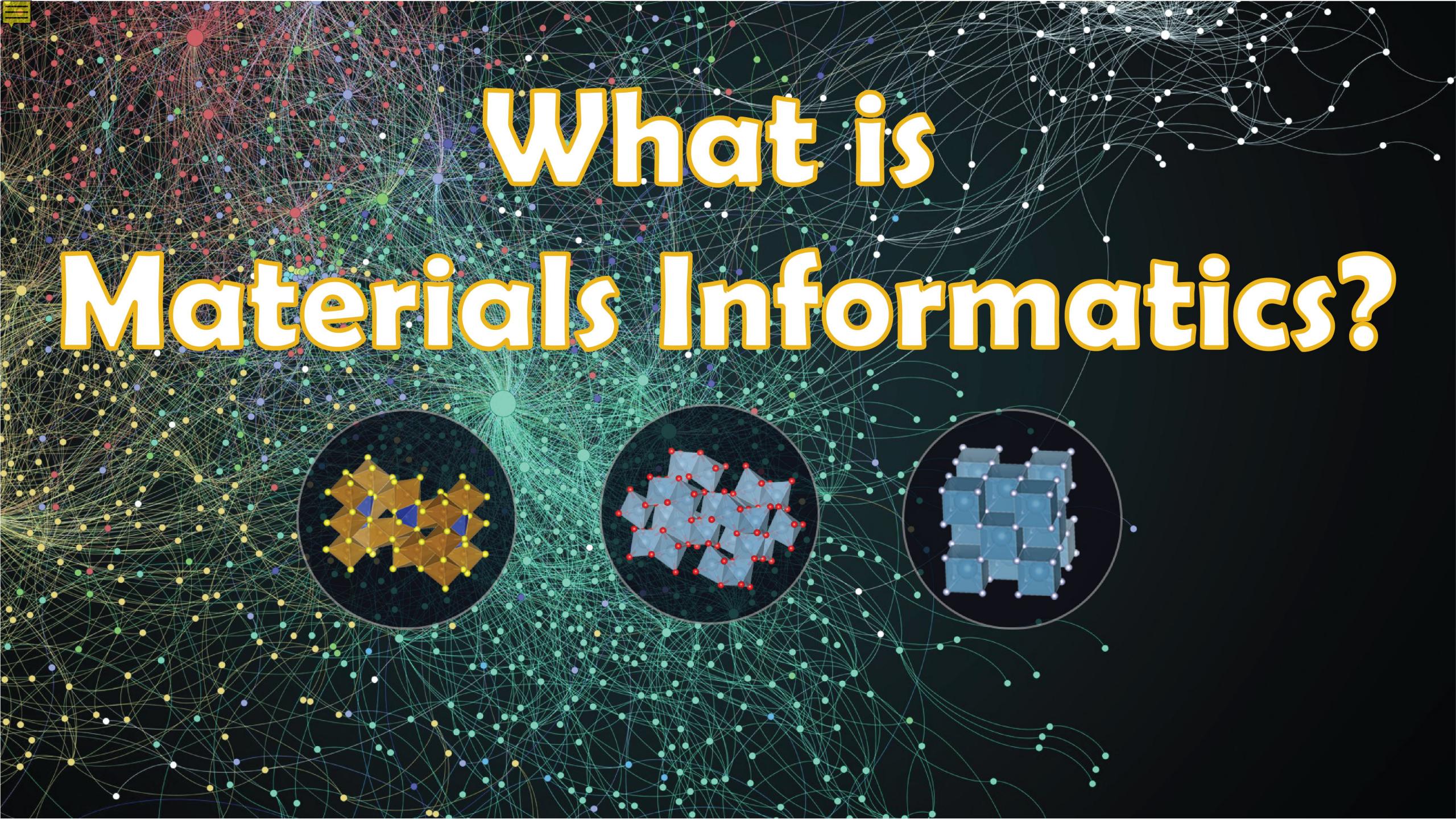


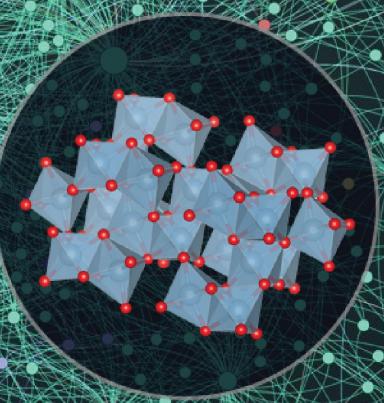
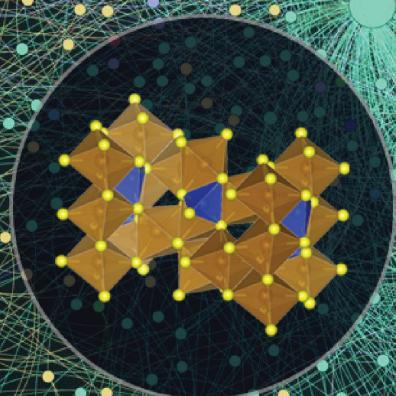
Materials Informatics



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

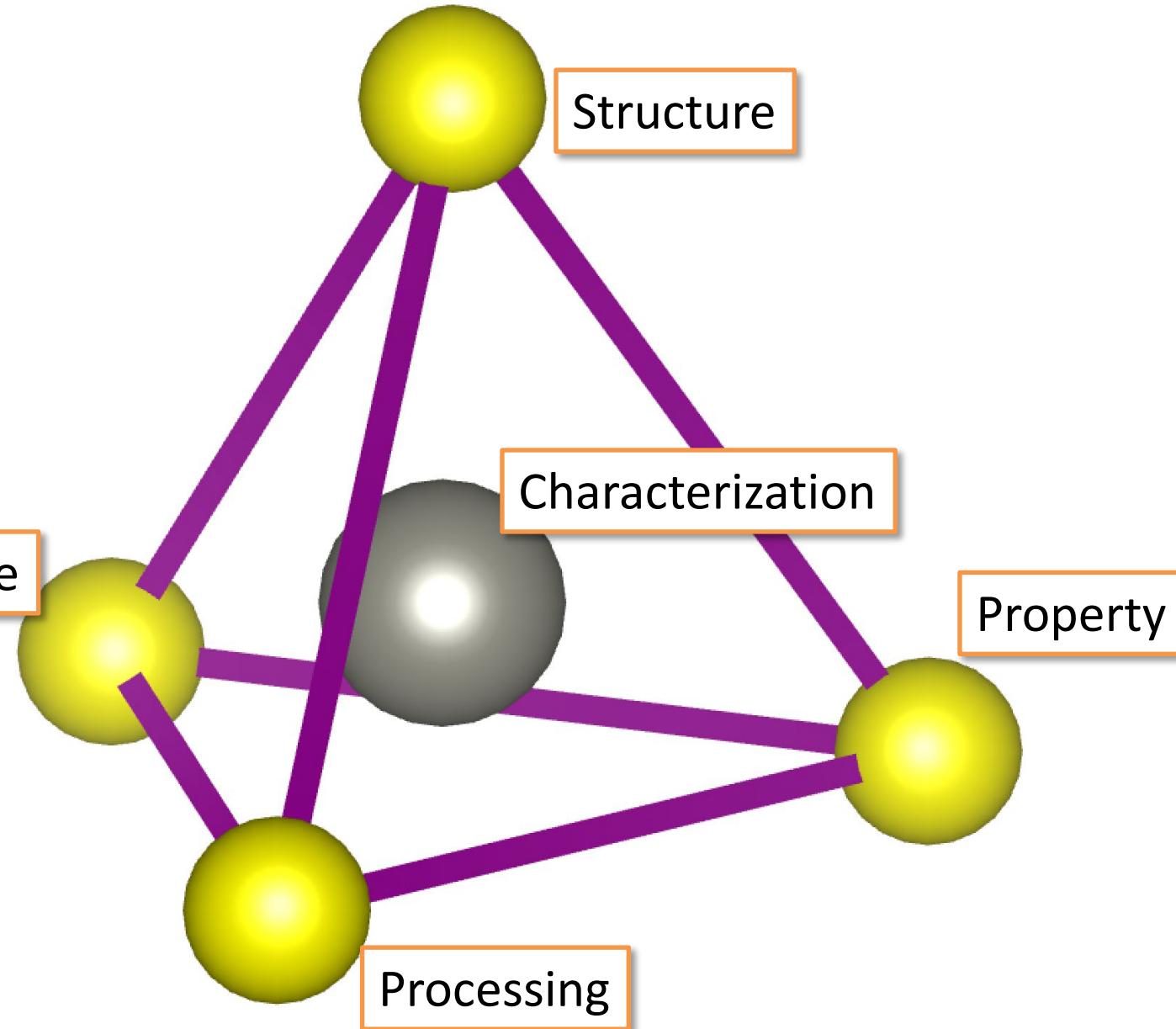


What is Materials Informatics?





Materials Informatics is data science applied to materials science





Materials Informatics is data science applied to materials science

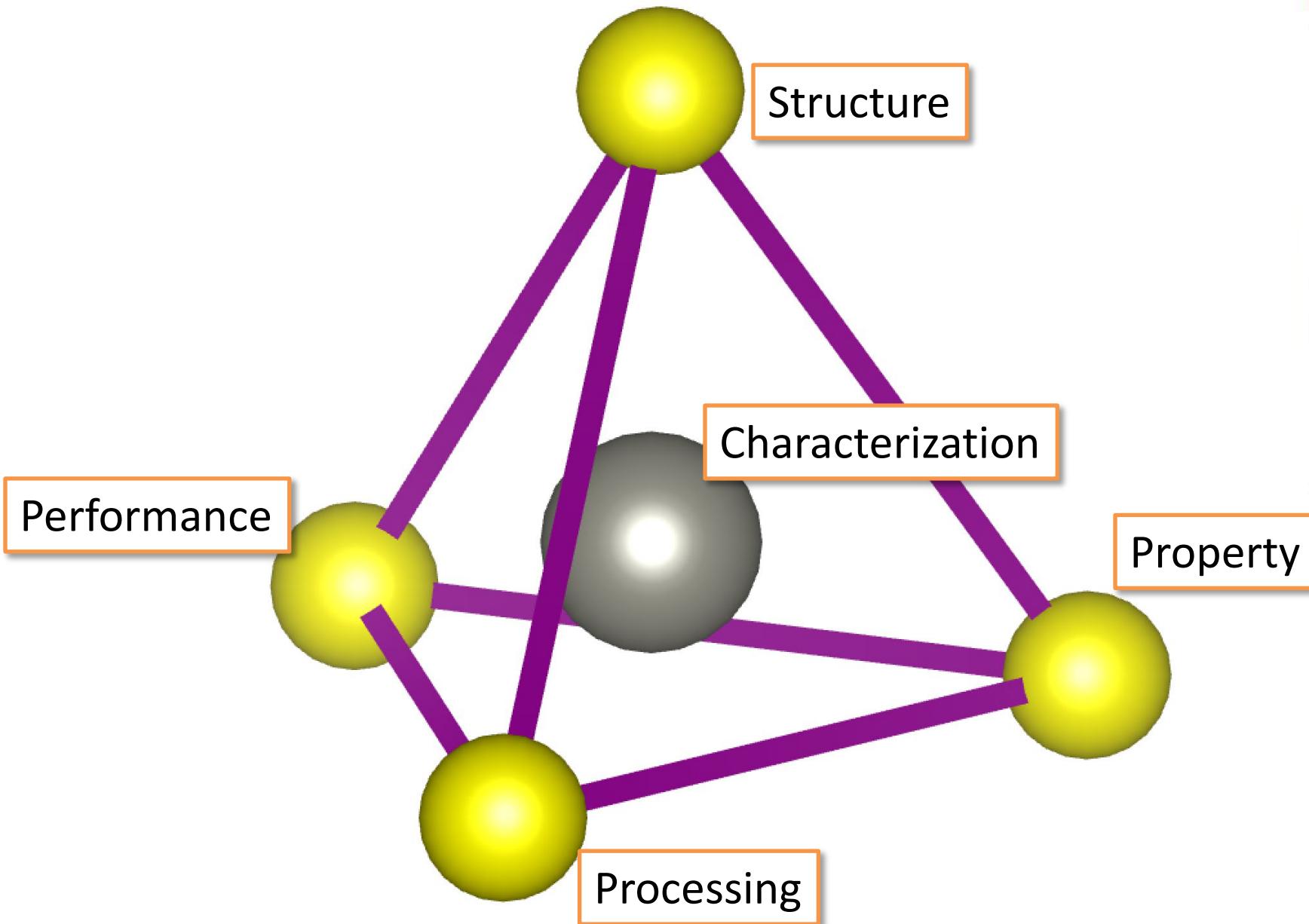
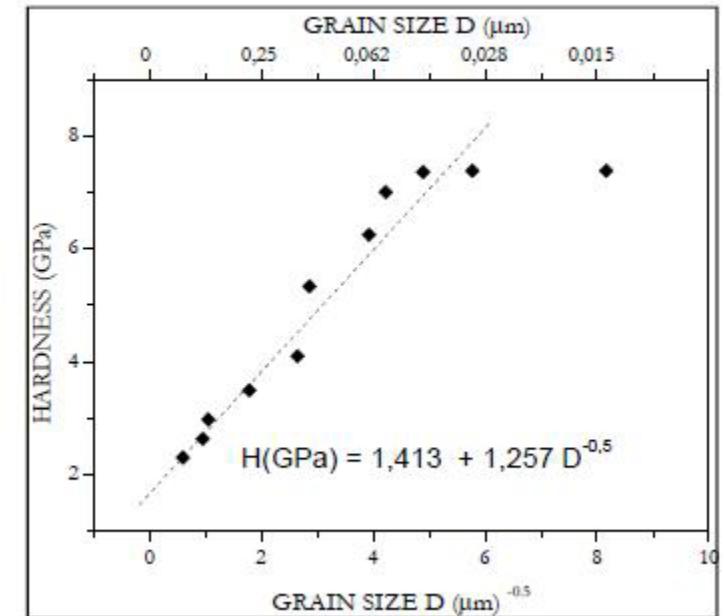


Figure 3. Hall-Petch ratio for 0.6%C steel





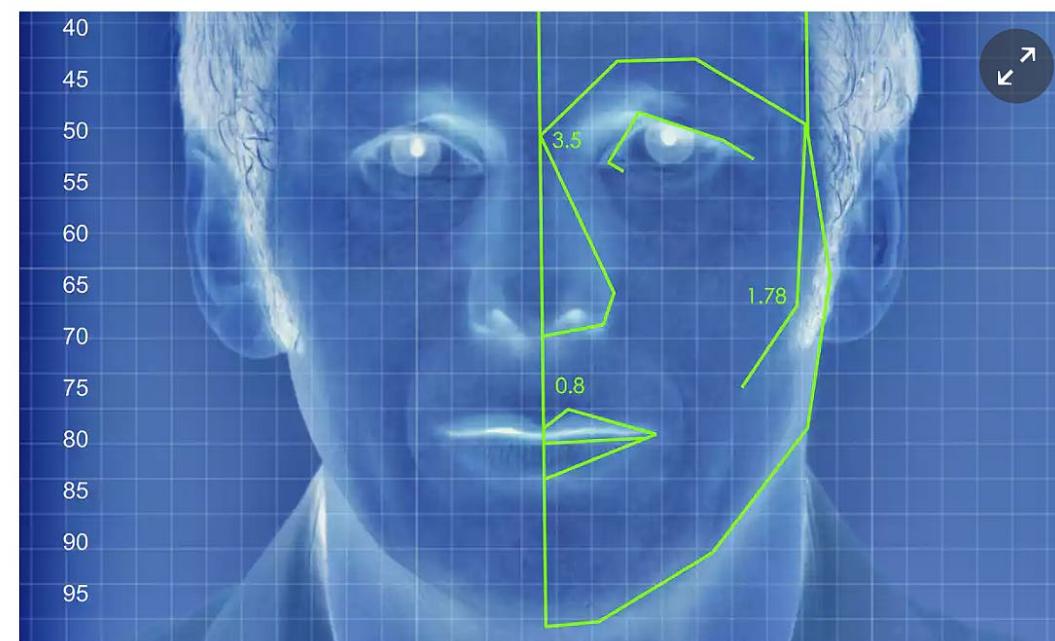
ML can extract highly complex trends in data!

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



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

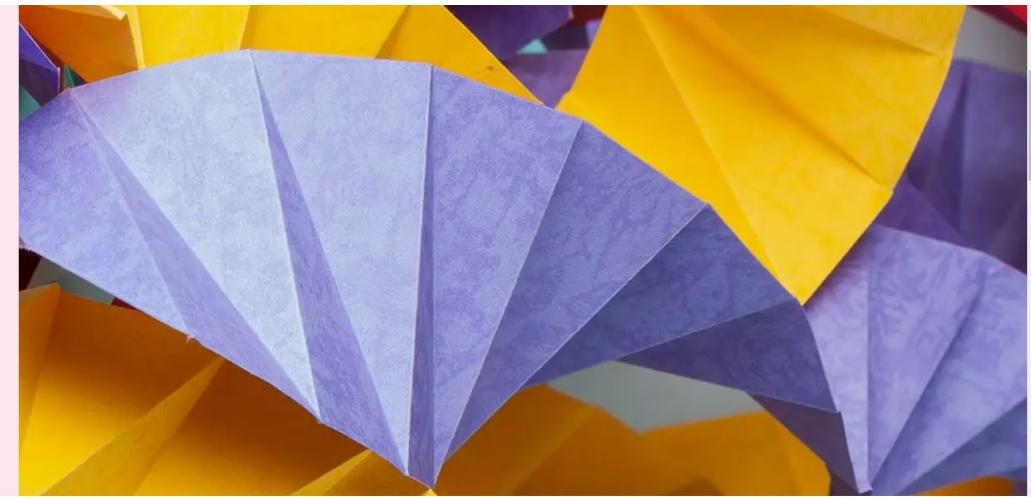
30 NOV 2020

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

SHARE



AUTHORS



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



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

materialstoday

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... 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

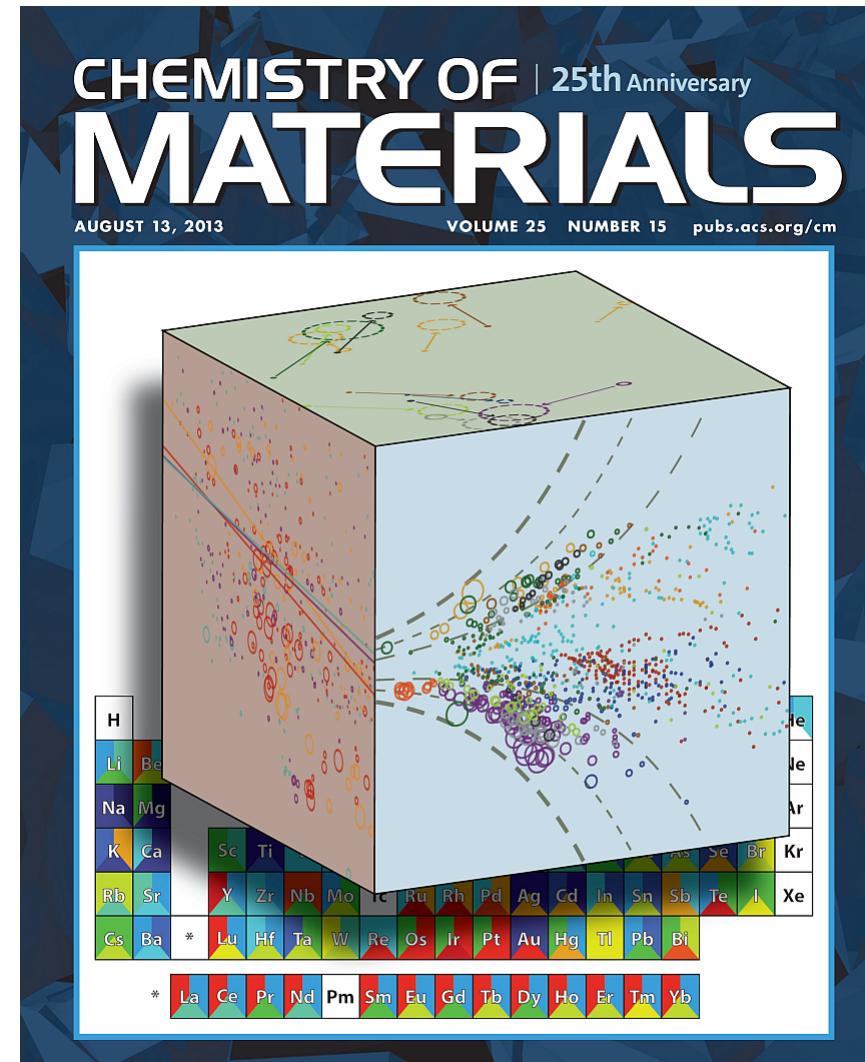
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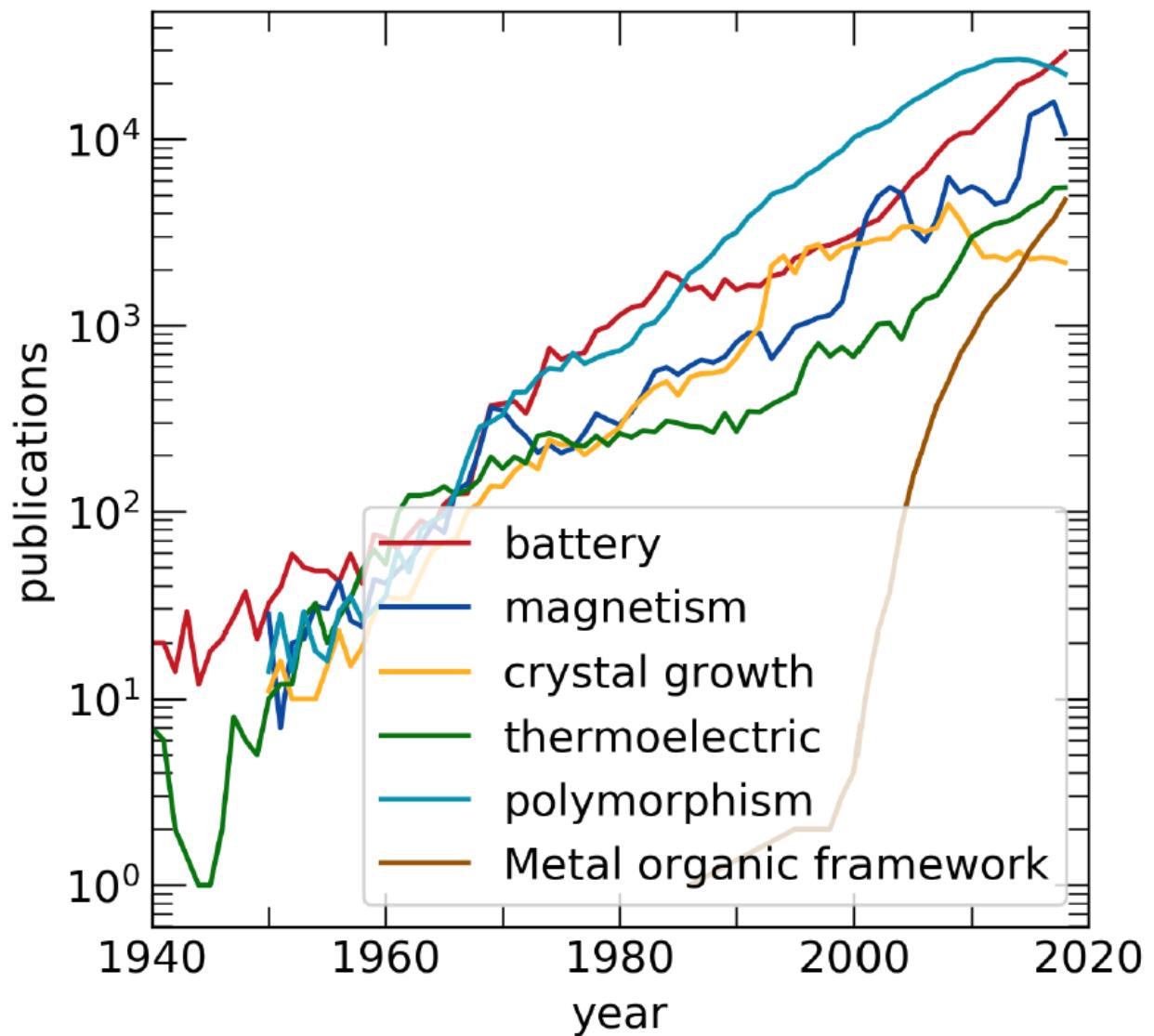
We initially used “big data” to write analytical reviews



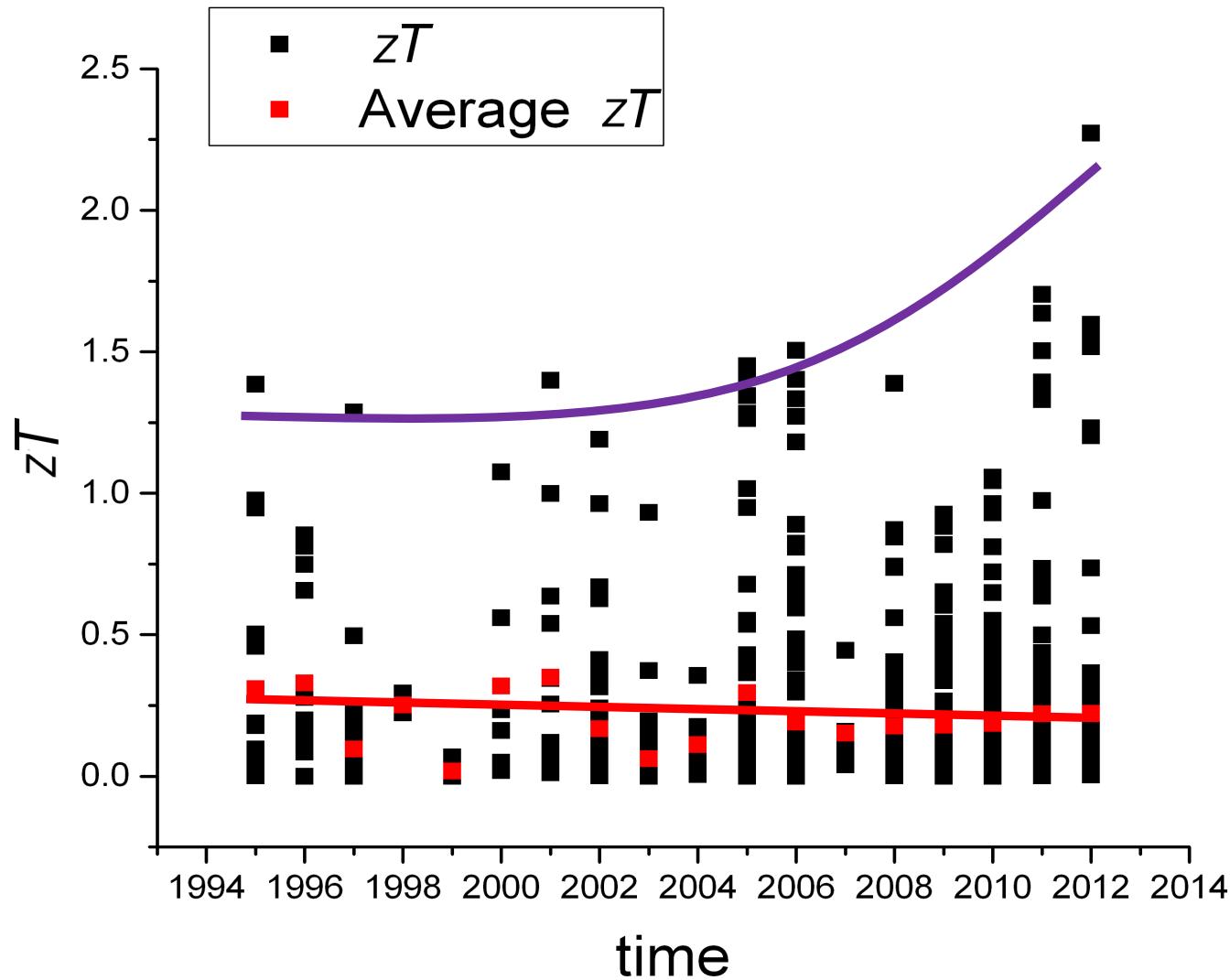
- Sparks et al. (2016) *Script. Mat.*
Gaultois et al. (2013) *Chem Mat.*
Ghadbeigi et al. (2016) *Energy Environ. Sci.*
Gaultois et al. (2016) *APL Mat.*



Why do we need data-driven materials science?



Most materials improvements are incremental



Breakthroughs are the uncommon exception

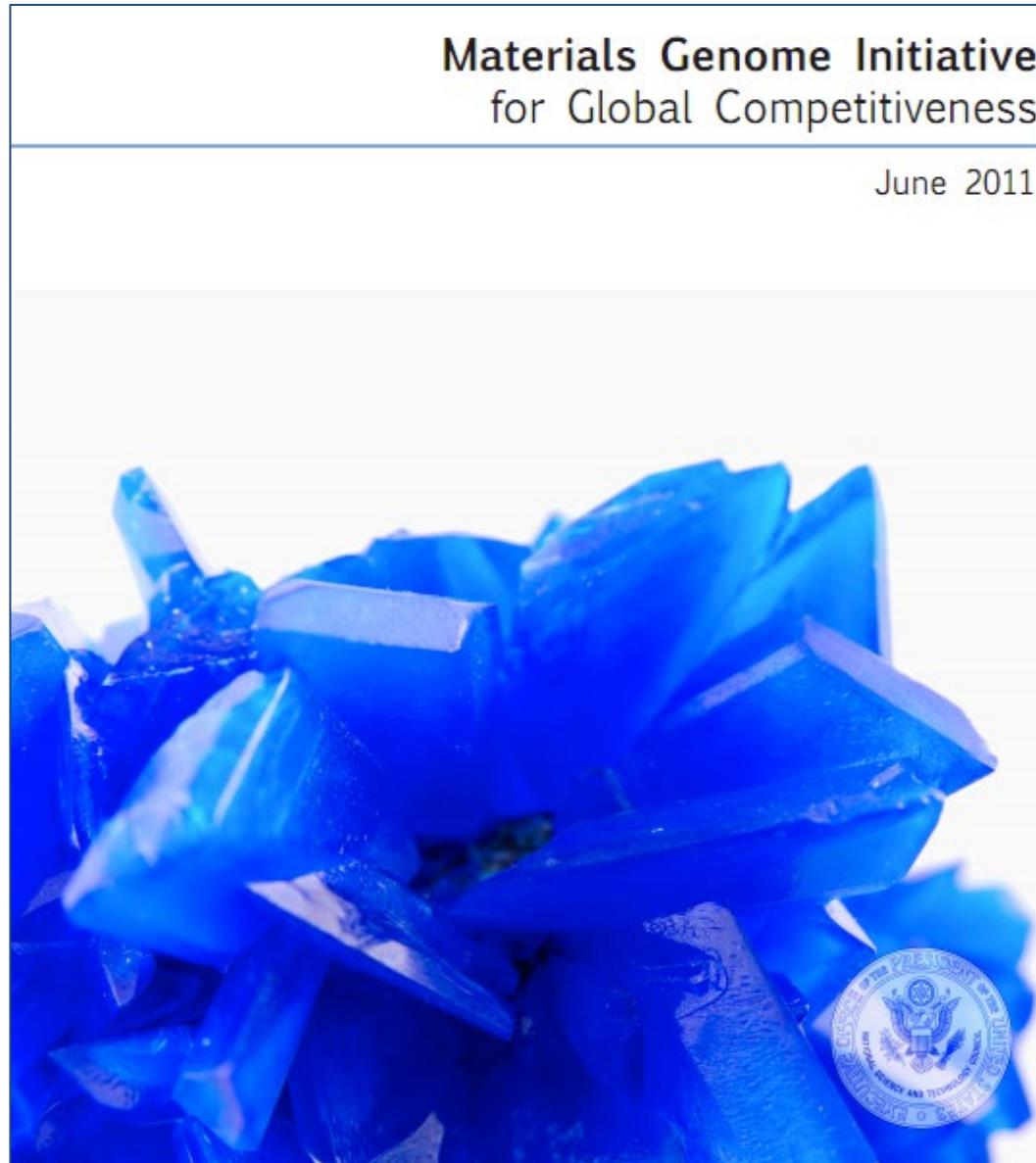


Useful relationships can be learned from data directly!



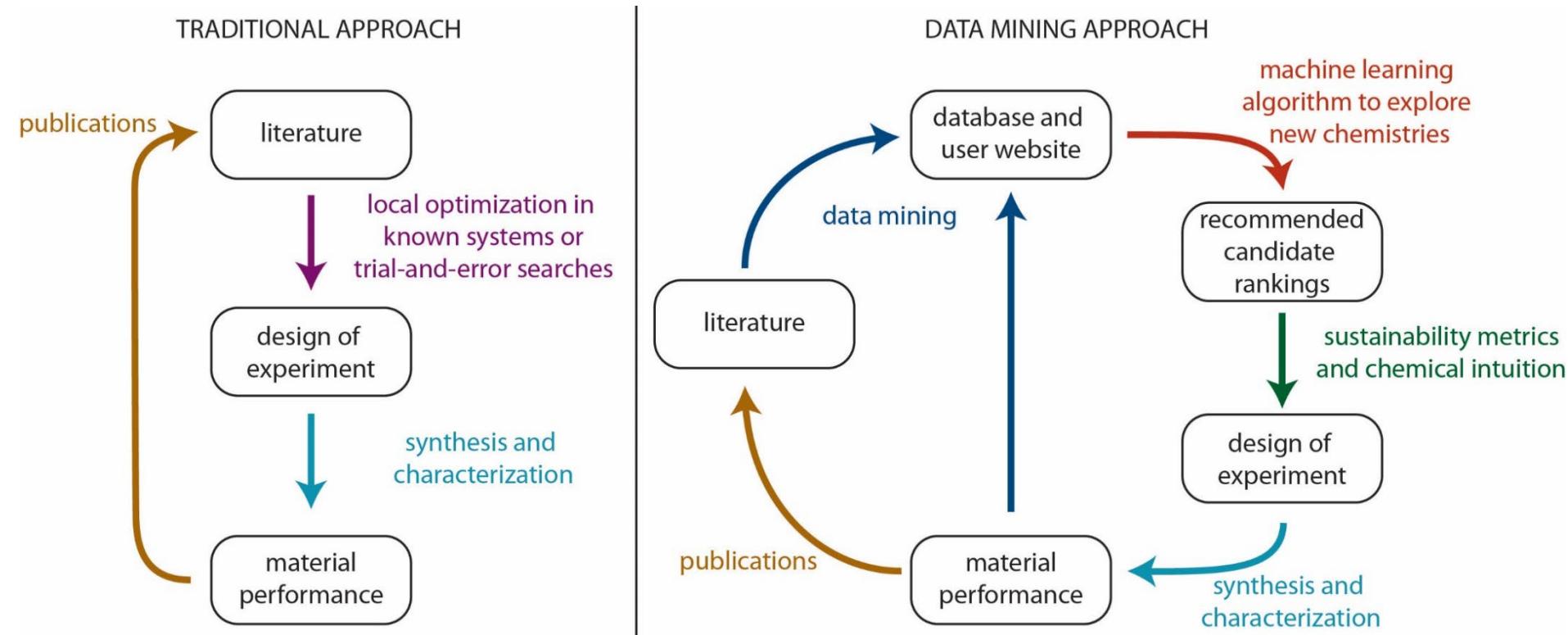


Are there “materials genes” responsible for desired behavior?



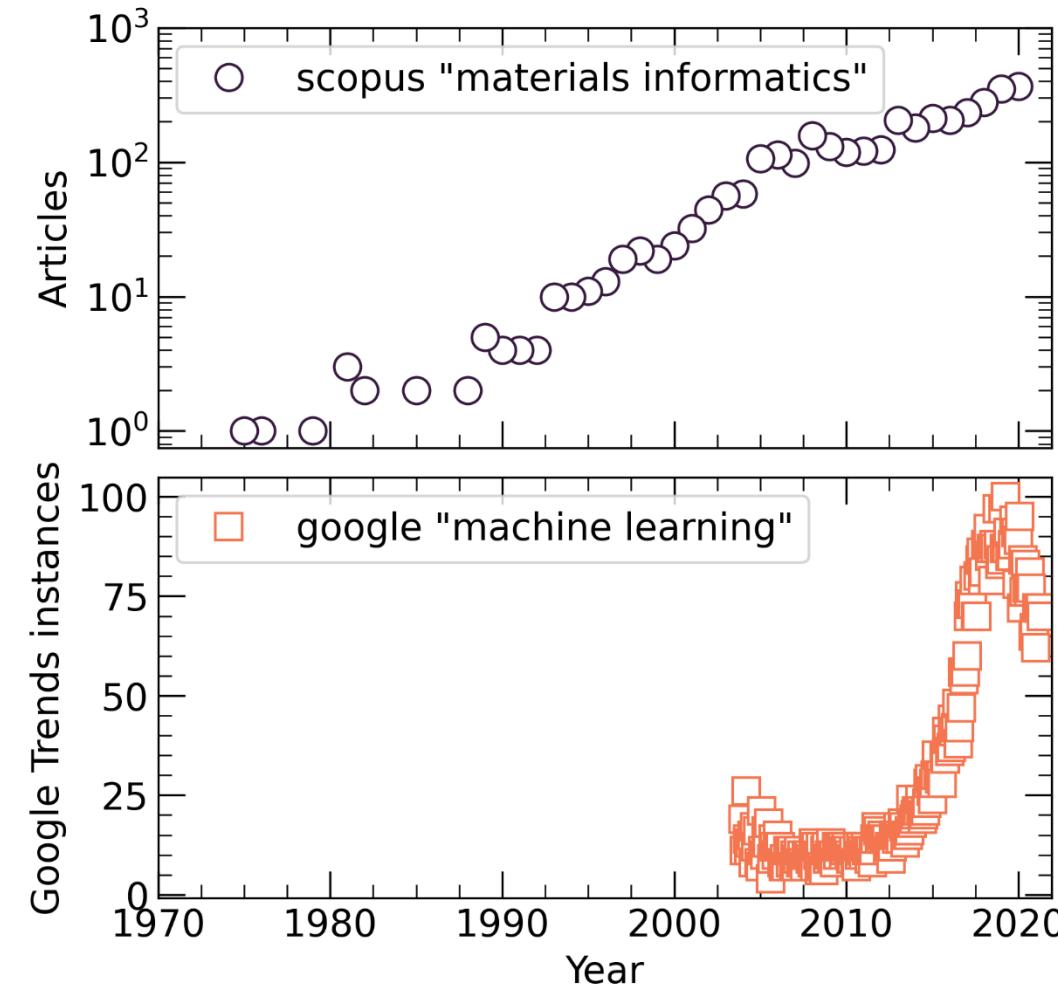
- Equip the next generation workforce
- Enable a paradigm shift in materials development
- Integrate experiments, computation, and theory
- Facilitate access to materials data

New tools of discovery are needed for “chemical whitespace”

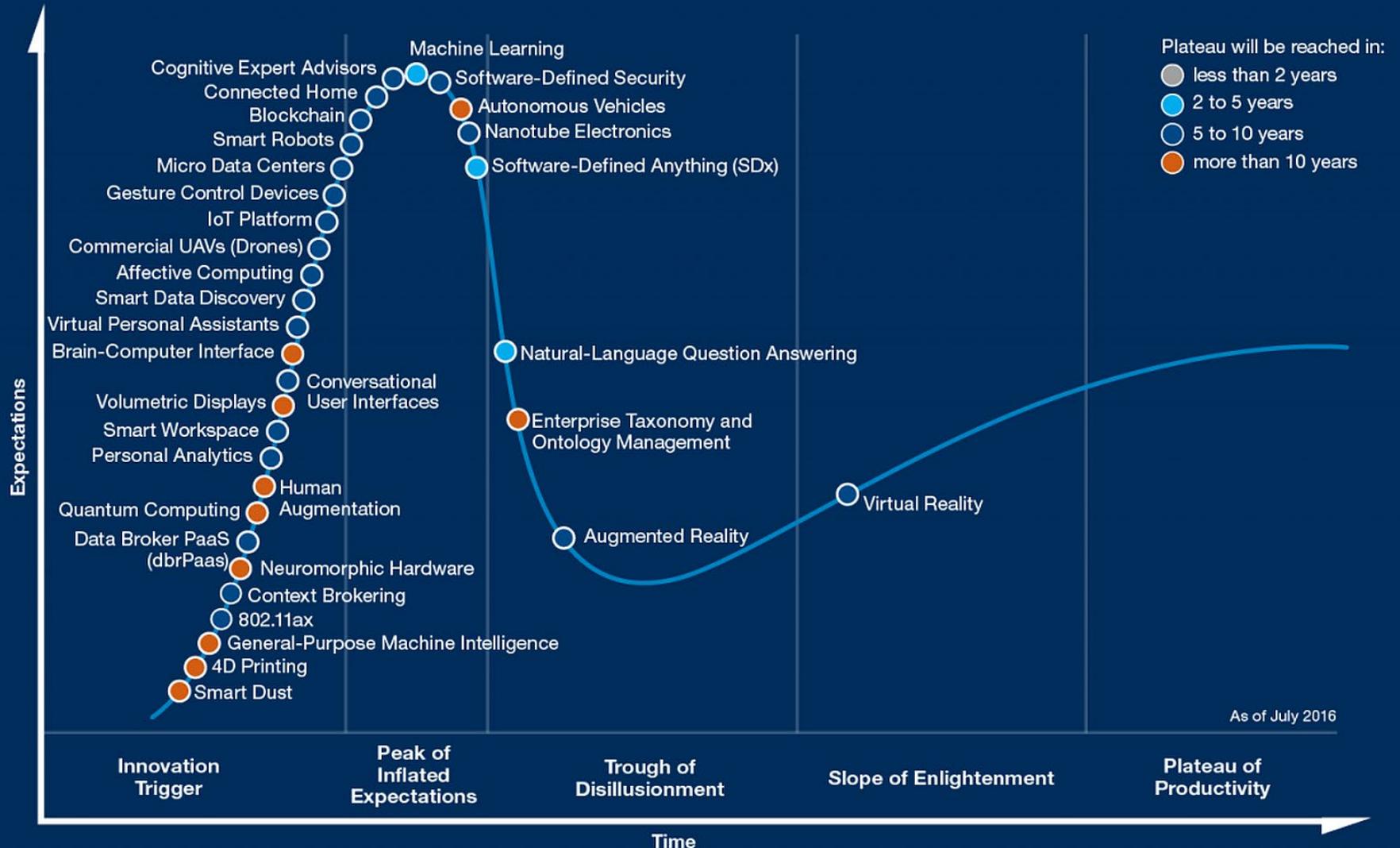




Is materials informatics a passing fad, or here to stay?



Gartner Hype Cycle for Emerging Technologies, 2016



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?

