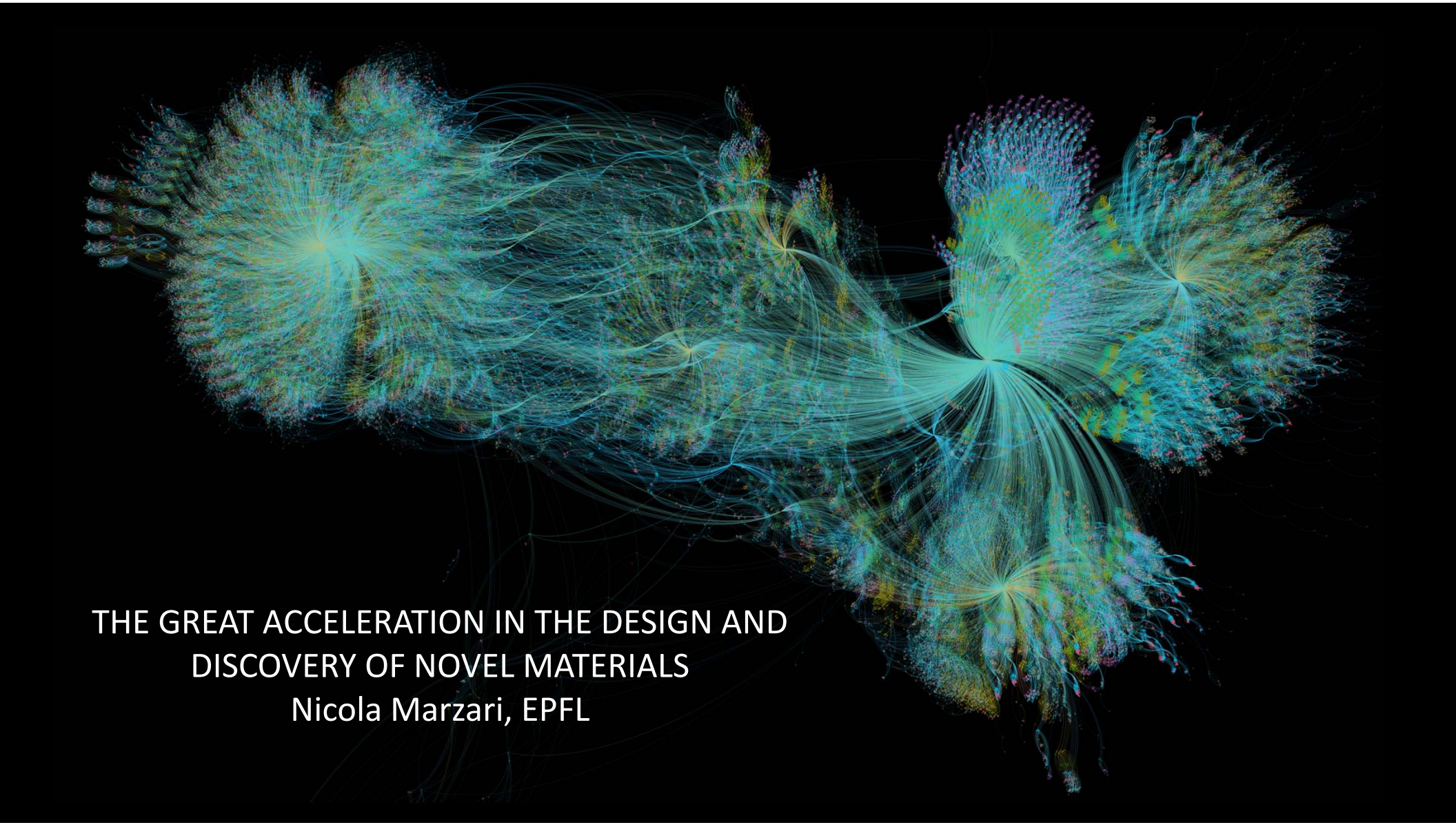


THE GREAT ACCELERATION IN THE DESIGN AND DISCOVERY OF NOVEL MATERIALS

Nicola Marzari, EPFL

THE RISE OF MATERIALS SCIENCE

THE RISE OF MATERIALS SCIENCE

3 Technologies That Could Create Trillion-Dollar Markets Over the Next Decade

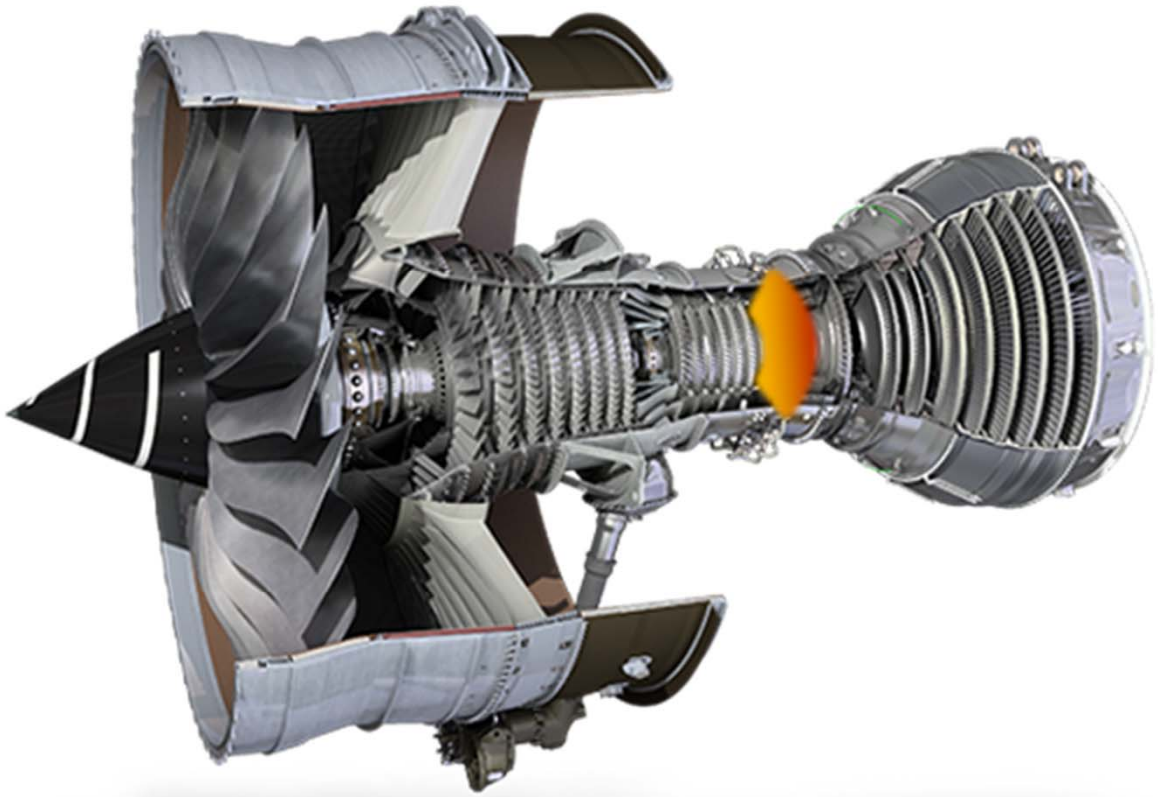
By Greg Satell Updated April 21, 2019 9:00 a.m. ET

Yet today, we're in the midst of a materials revolution. Powerful simulation techniques, combined with increased computing power and machine learning, are enabling researchers to automate much of the discovery process, vastly accelerating the development of new materials

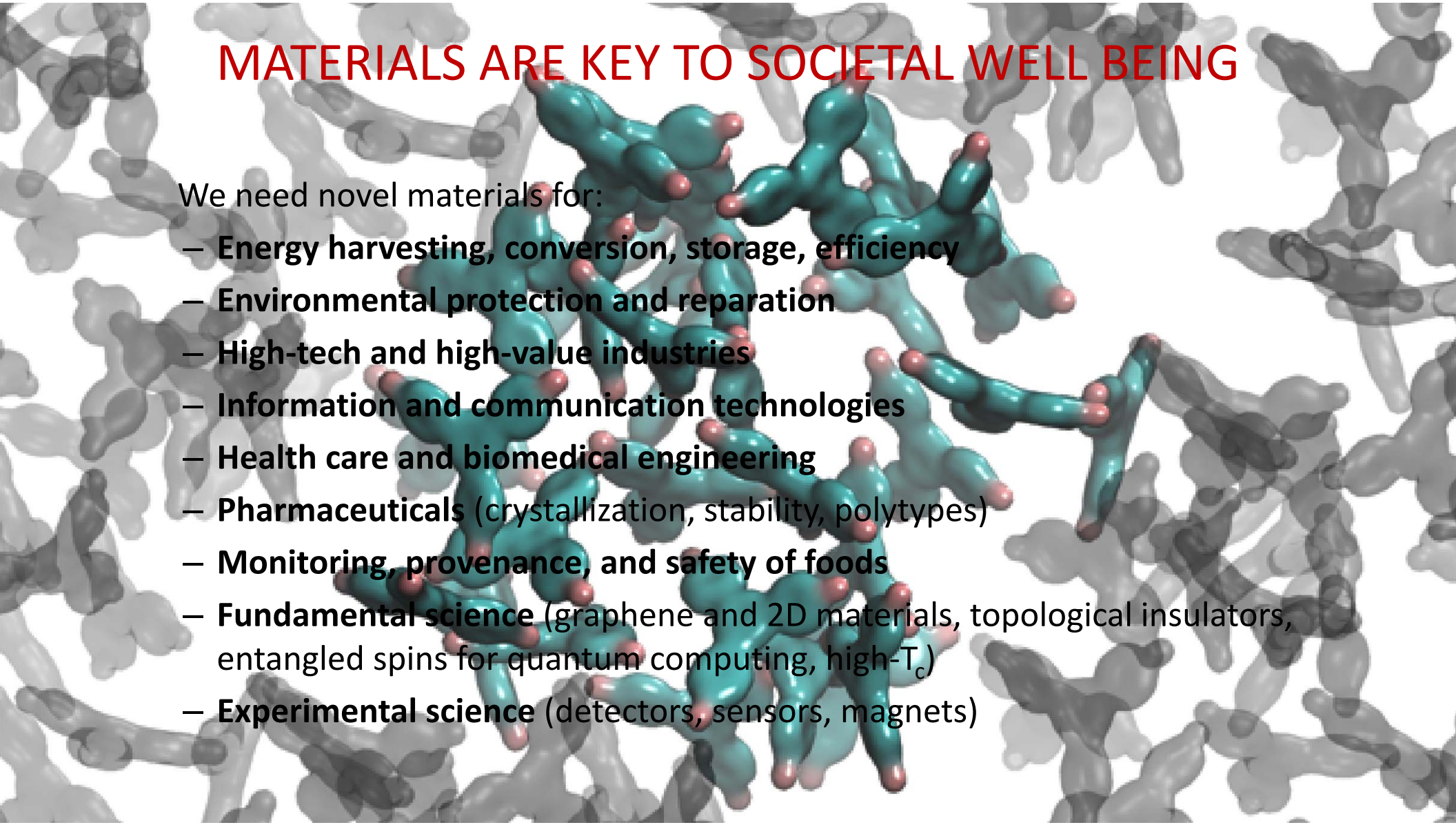
BARRON'S (April 2019)

A FEW EASY PIECES

NEXT TIME YOU FLY



MEET CLARA AND FRITZ

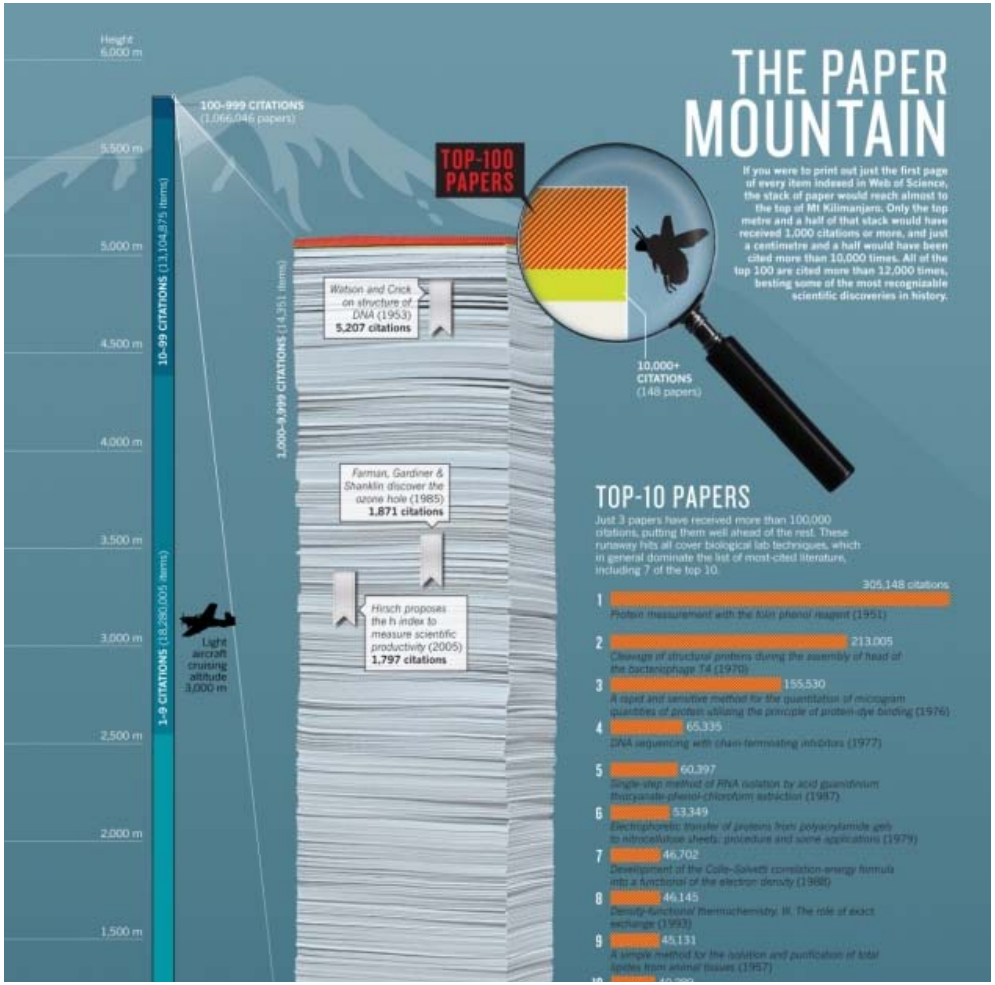


MATERIALS ARE KEY TO SOCIETAL WELL BEING

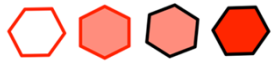
We need novel materials for:

- **Energy harvesting, conversion, storage, efficiency**
- **Environmental protection and reparation**
- **High-tech and high-value industries**
- **Information and communication technologies**
- **Health care and biomedical engineering**
- **Pharmaceuticals** (crystallization, stability, polytypes)
- **Monitoring, provenance, and safety of foods**
- **Fundamental science** (graphene and 2D materials, topological insulators, entangled spins for quantum computing, high-T_c)
- **Experimental science** (detectors, sensors, magnets)

THE RISE OF QUANTUM-MECHANICAL SIMULATIONS



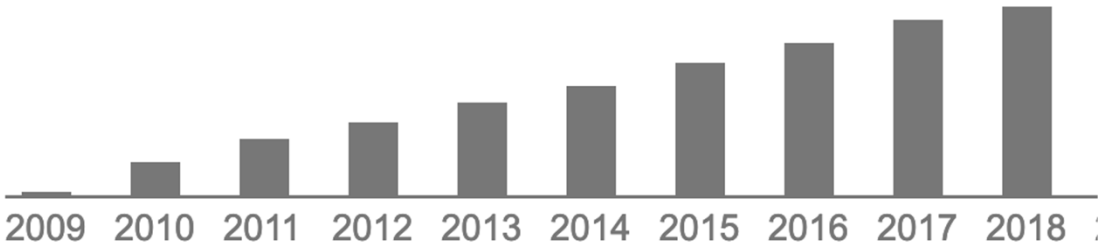
Density-functional theory as the most cited field ever across science, medicine, engineering… [Nature, 2014]



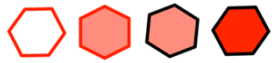
SOFTWARE AS MAJOR INFRASTRUCTURE

QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials

Total citations Cited by 12963



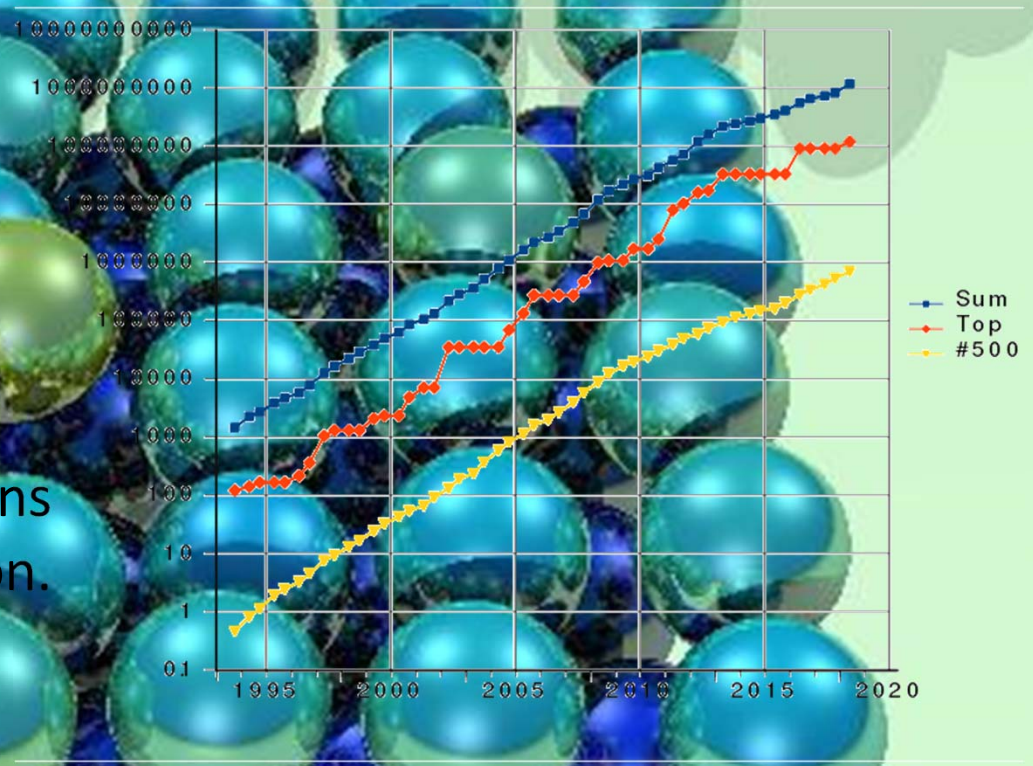
In 2019 there will be ~3000 scientific papers published using a single, free, European open-source code, supported by the H2020 MaX Centre of Excellence for Materials Design at the eXascale



THE BUSINESS MODEL

A calculation that took
one year in 1990
would take
one second in 2019
(33-million-fold increase).

And this is just with bits: neurons are in, and qubits on the horizon.
21st-century science will be computational.



MATERIALS MODELLING

The frontiers and the challenges

Materials simulations have become a dominant force in the world of science and technology. The intellectual challenges lying ahead to sustain such a paradigm shift are discussed.

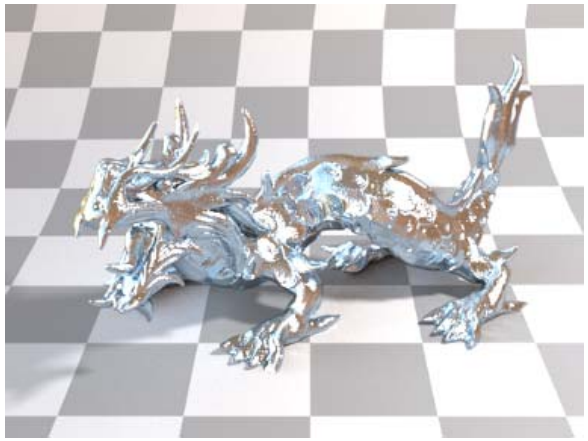
Nicola Marzari

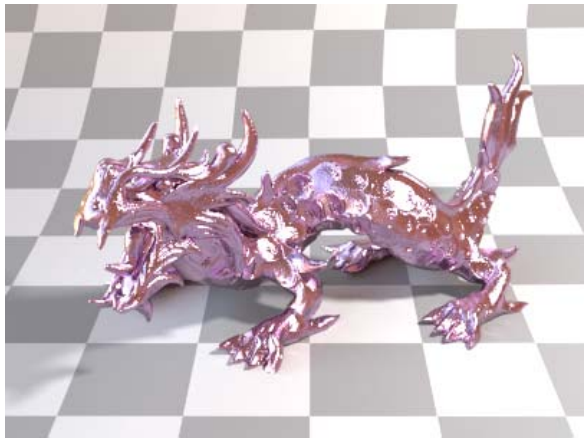
1) PREDICTIVE ACCURACY

2) REALISTIC COMPLEXITY

3) MATERIALS' INFORMATICS

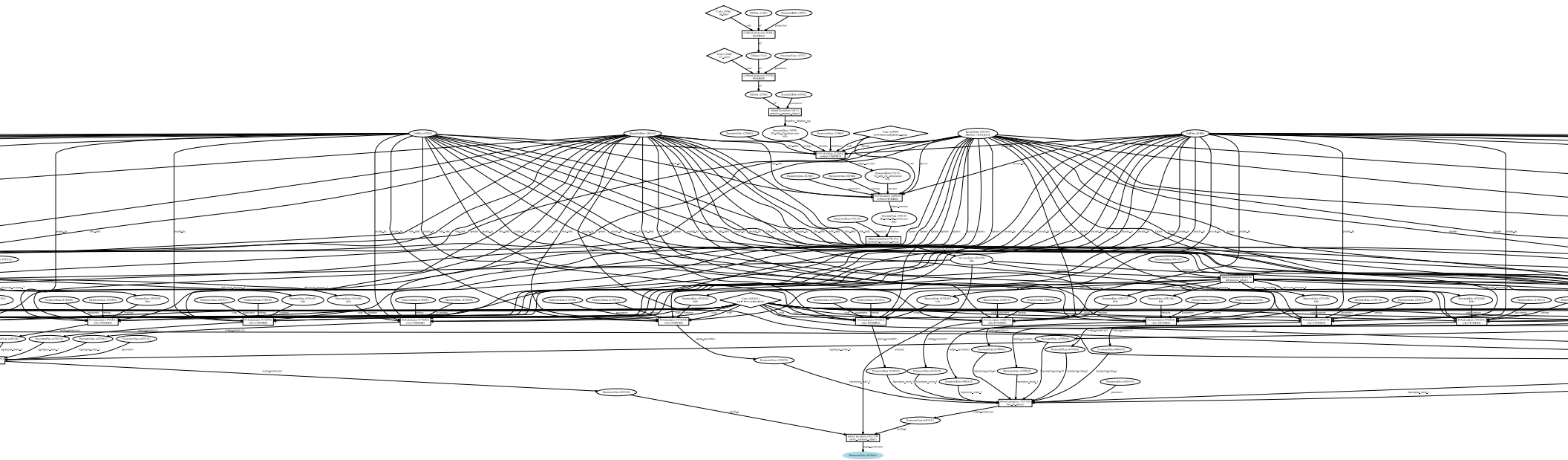
HOW WELL CAN WE REPRODUCE THE REAL WORLD?



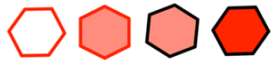



AUTOMATED, HIGH-THROUGHPUT, ON-DEMAND DATA

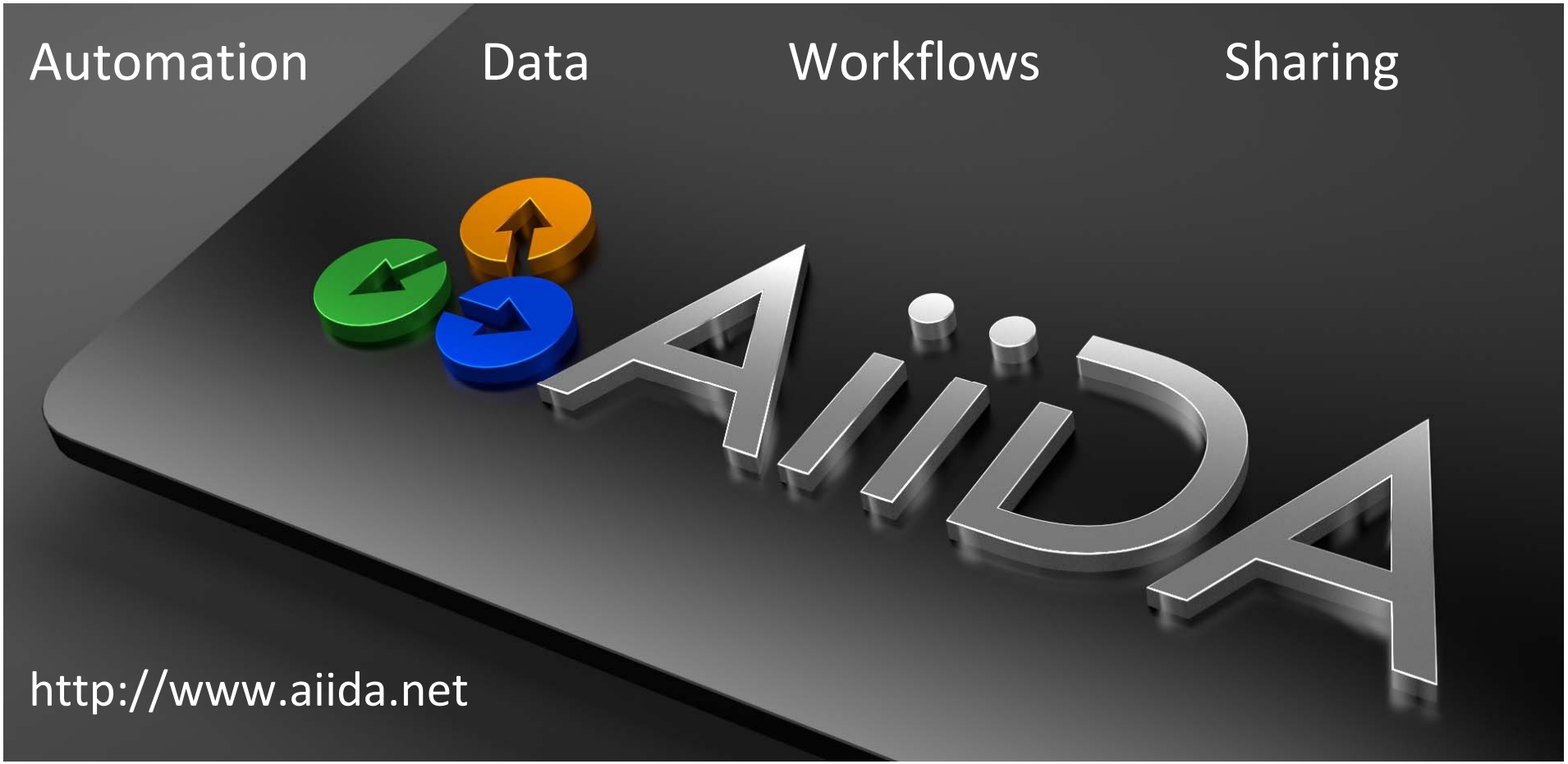
Input: Structure



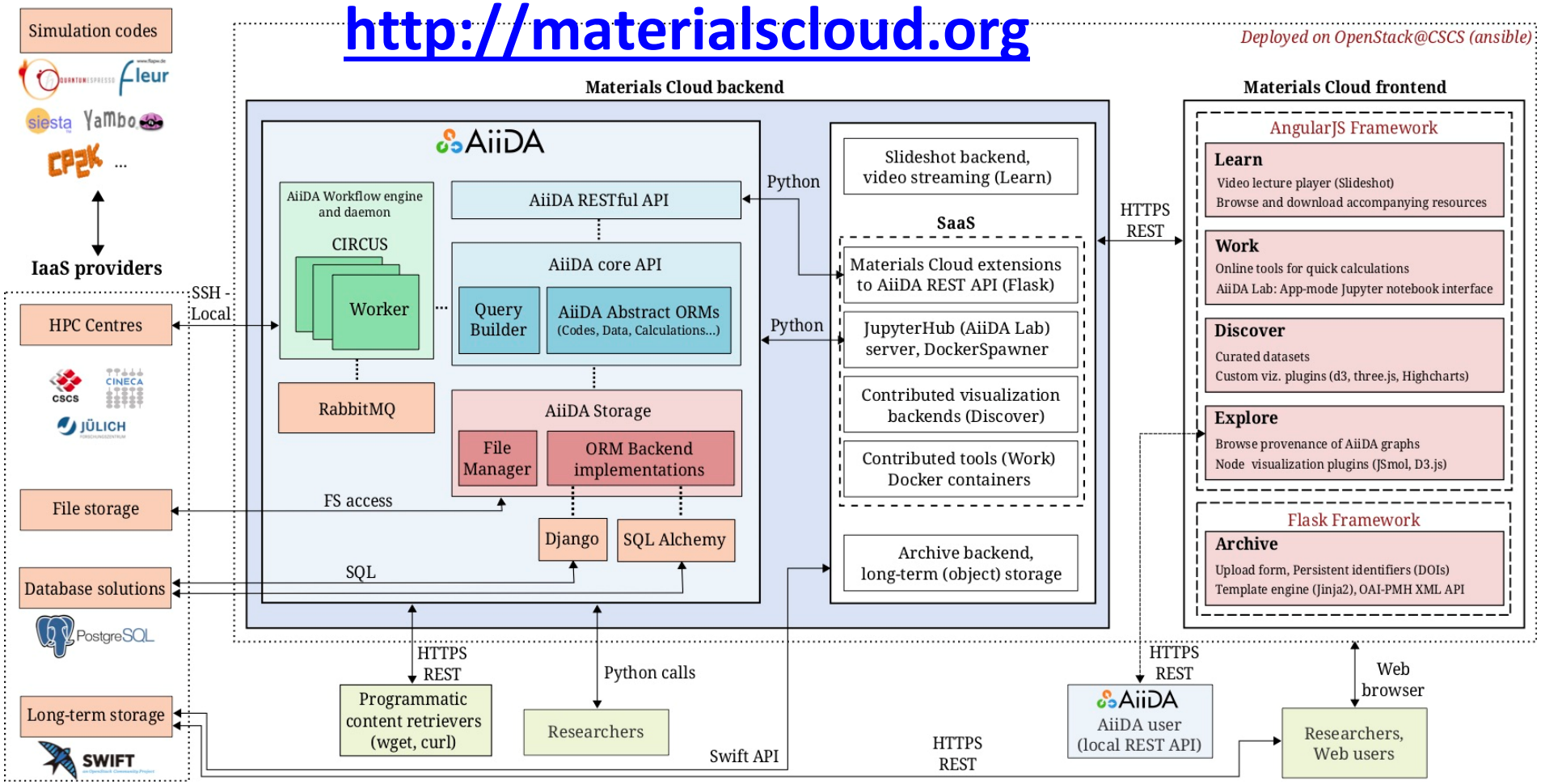
Output: Property



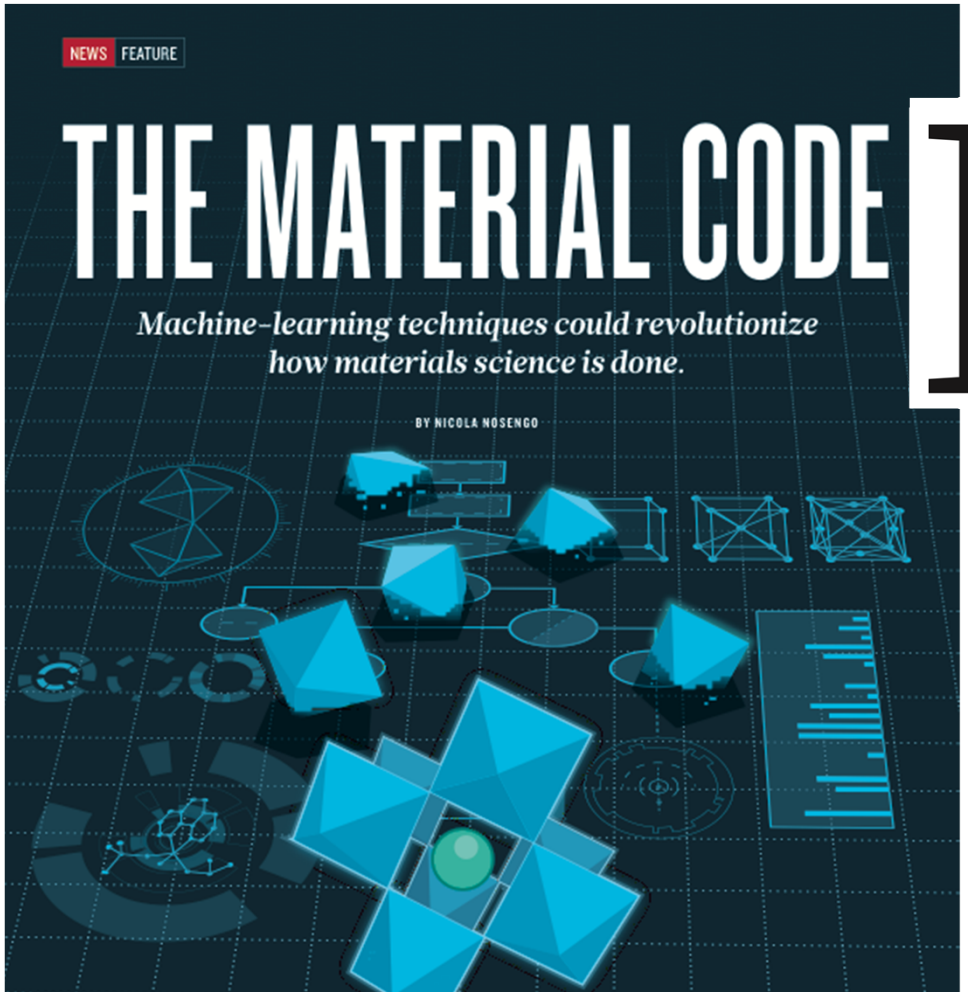
WE BUILT AN ENTIRE OPERATING SYSTEM FOR THIS



THE CONVERGENCE OF HPC, HTC, AND HPDA

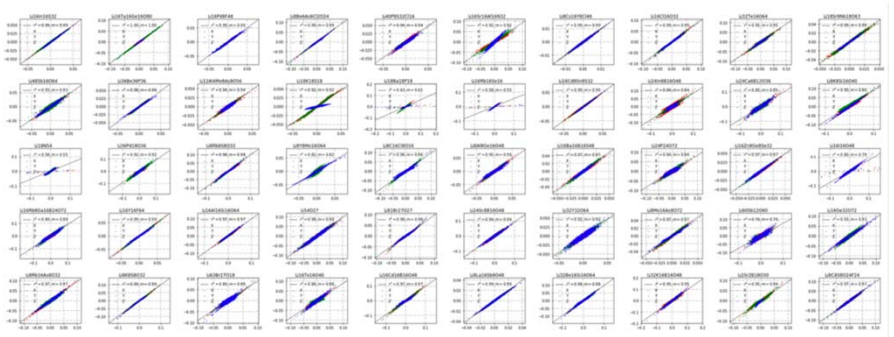


MACHINE LEARNING: FROM ONE MONTH TO ONE MINUTE



Nature, May 2016

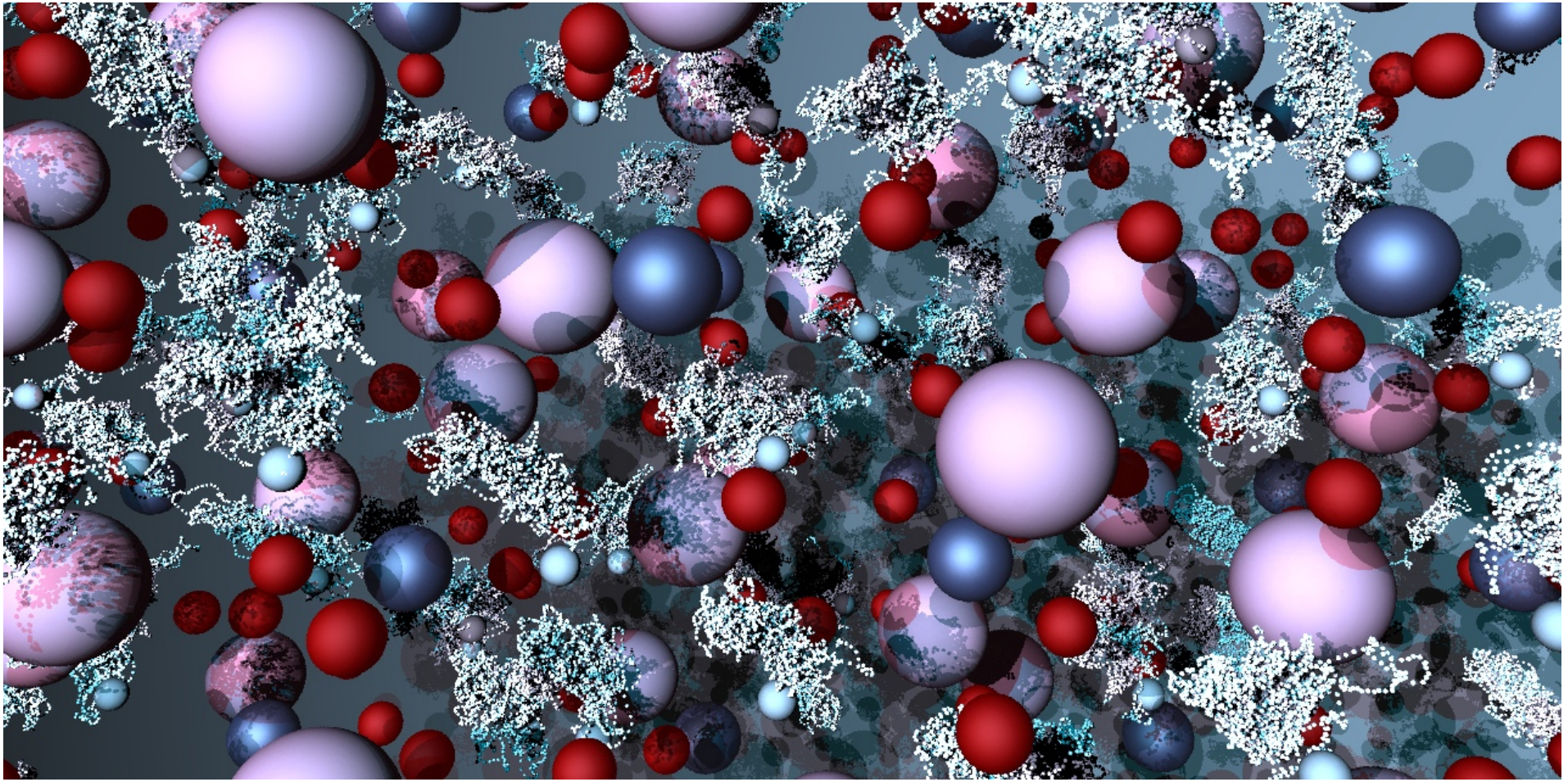
It's a strong contender for the geekiest video ever made: a close-up of a smartphone with line upon line of numbers and symbols scrolling down the screen. But when visitors stop by Nicola Marzari's office, which overlooks Lake Geneva, he can hardly wait to show it off. "It's from 2010," he says, "and this is my cellphone calculating the electronic structure of silicon in real time!"



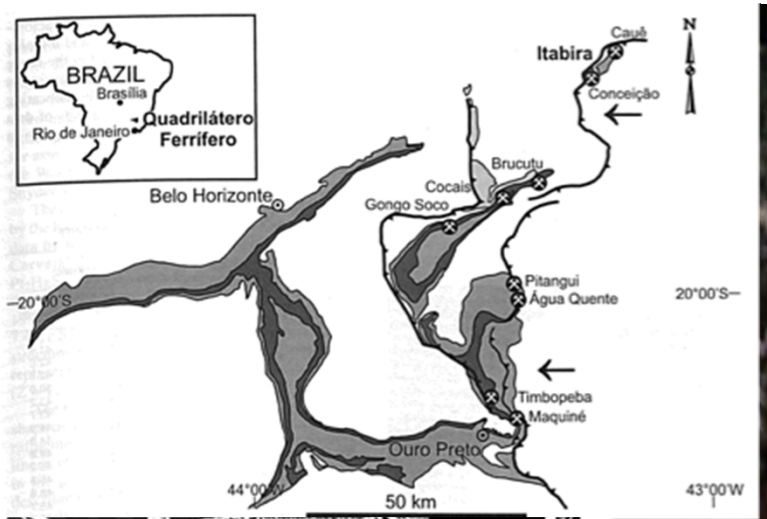
DEVELOPING SAFE, MORE POWERFUL BATTERIES

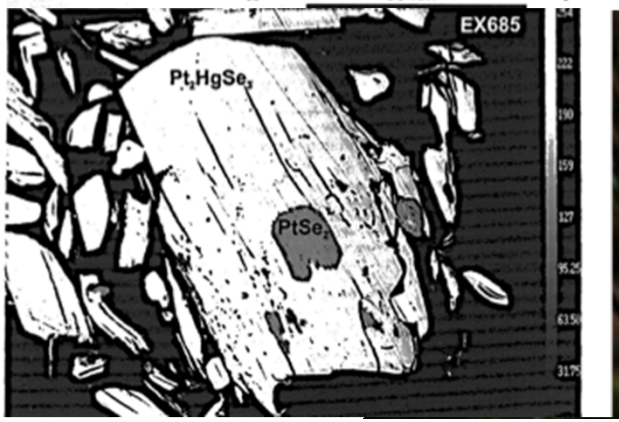
Energy density of a battery is one-tenth of a TNT bomb!

NEW SOLID STATE CONDUCTORS

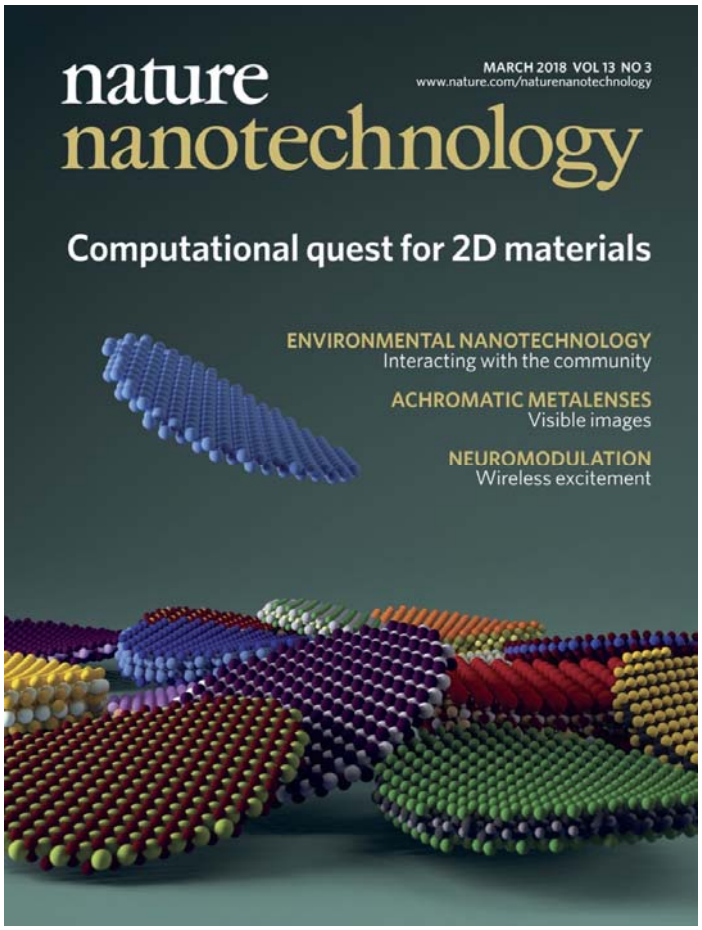


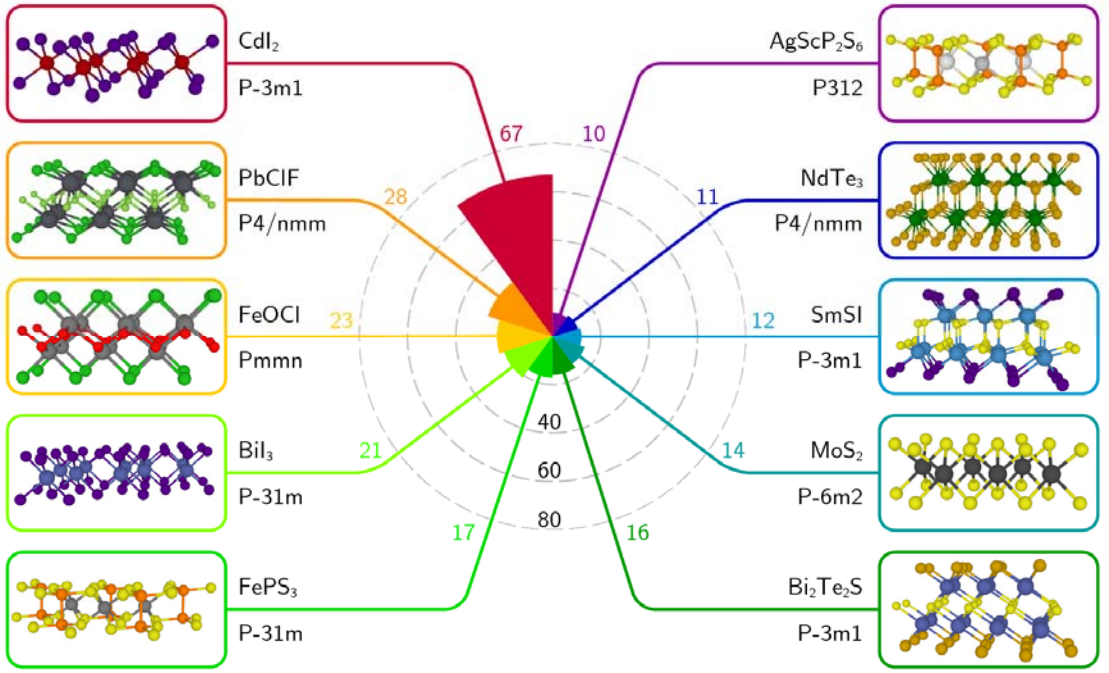
A ROOM-TEMPERATURE TOPOLOGICAL INSULATOR

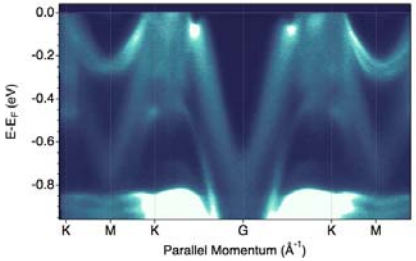


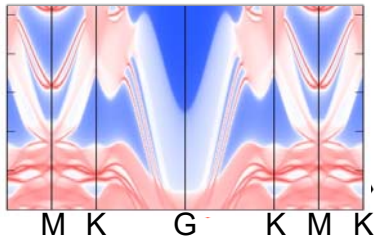


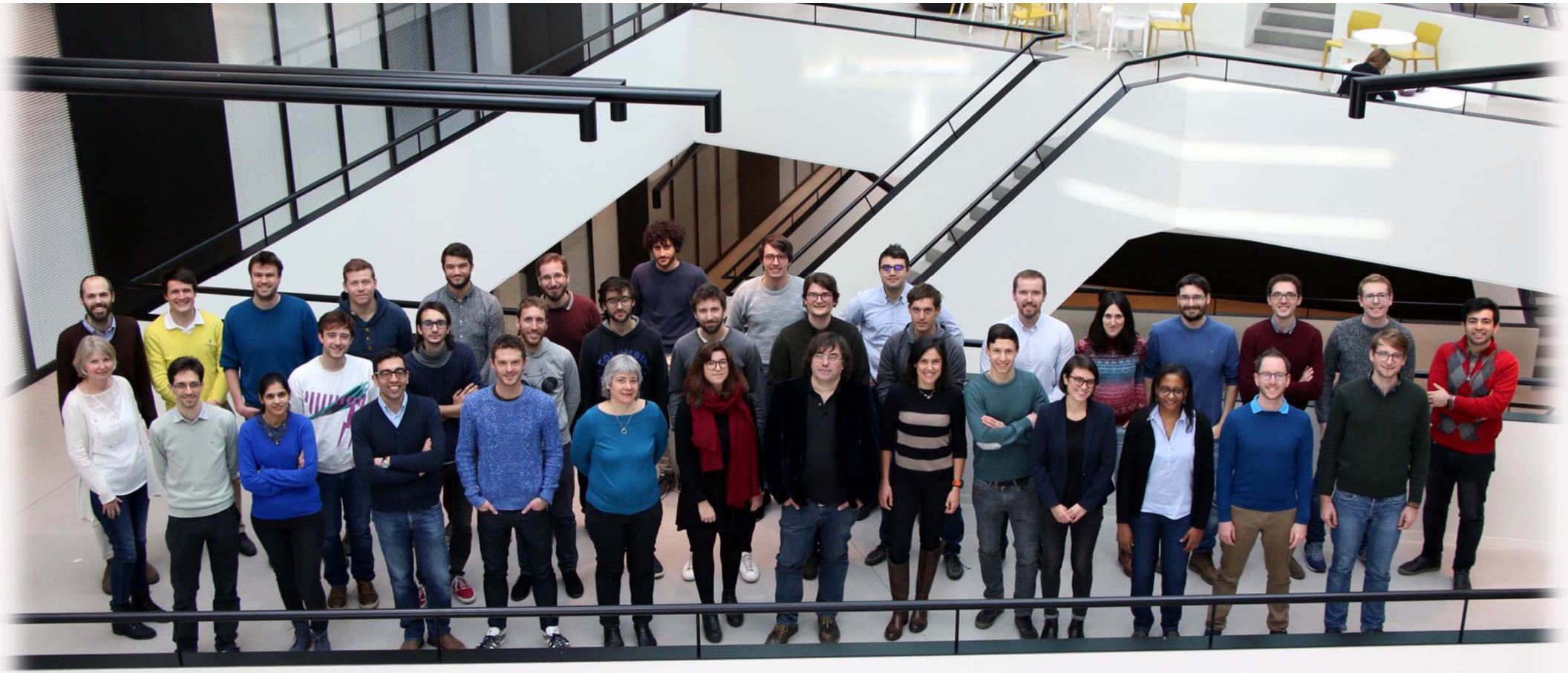
2000 NOVEL TWO DIMENSIONAL MATERIALS











http://nccr-marvel.ch/ (2014-2026)
http://max-centre.eu/ (2015-2021)

MATERIALS CLOUD

EMMC

CONCLUSIONS

1. Materials enable the technologies that sustain our economy, our lives, our society
2. We are changing the entire paradigm of materials design and discovery (QM simulations, ML/data, neuro/qubit)
3. Physical infrastructure ceases to be the limit of exploration
4. Computational science will be foundational and pervasive in this century (yet we do not have a development/support model)