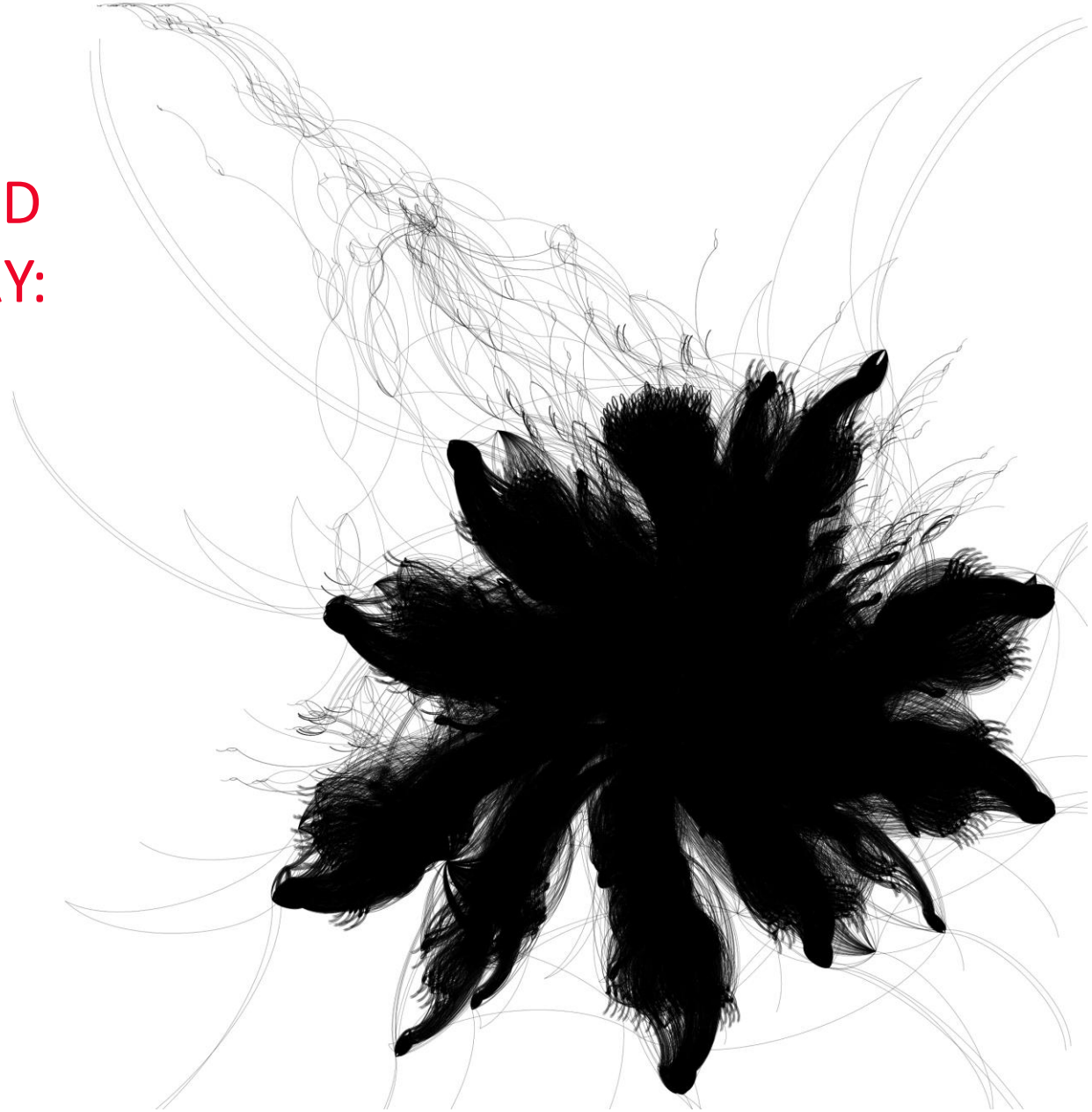
HIGH-THROUGHPUT SCREENING AND MATERIALS MODELLING IN INDUSTRY: SUCCESS CASES FROM MAX

Nicola Marzari, EPFL



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)

MAX DRIVING THE EXASCALE TRANSITION

MATERIALS MAKE TECHNOLOGY POSSIBLE

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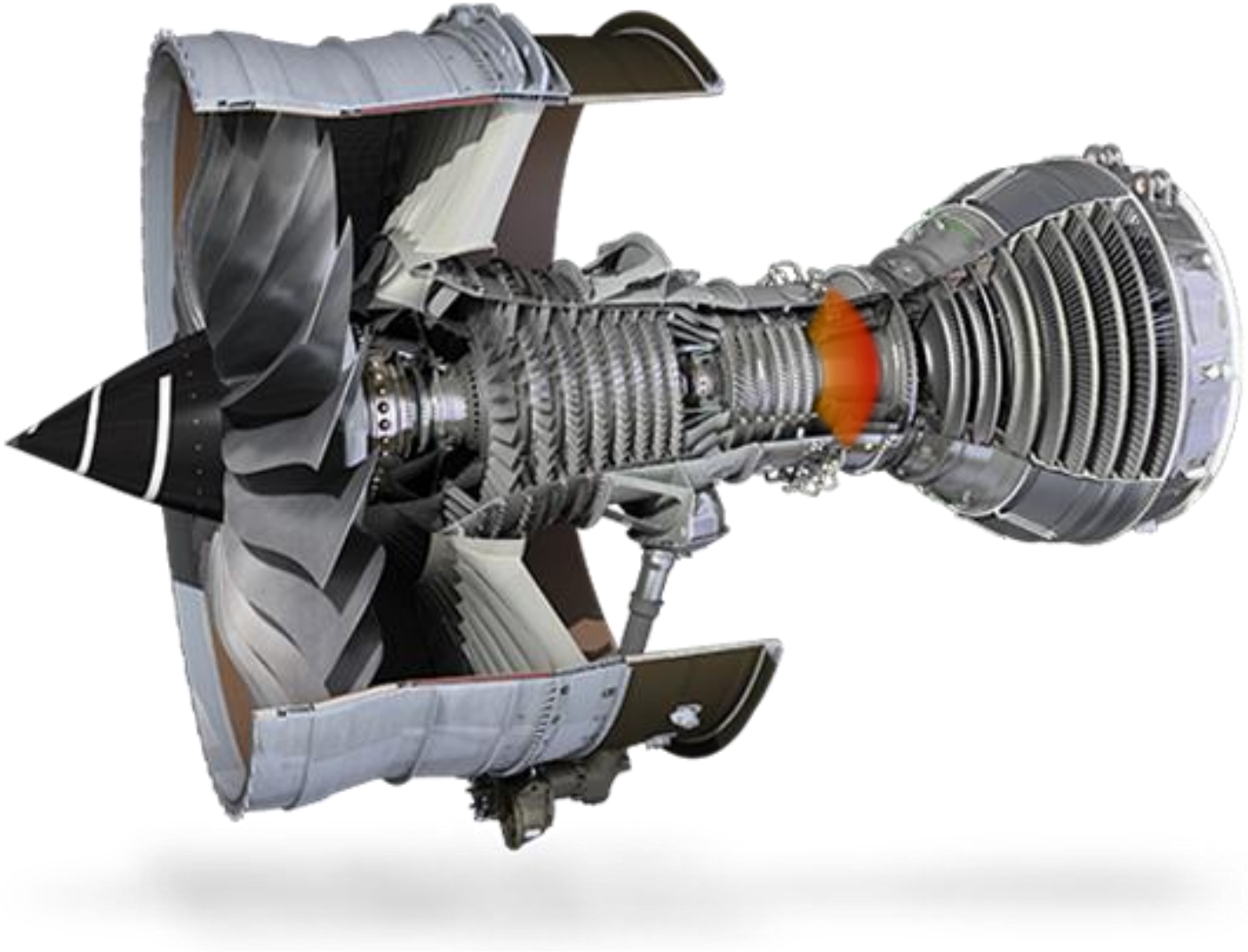
NEXT TIME YOU FLY



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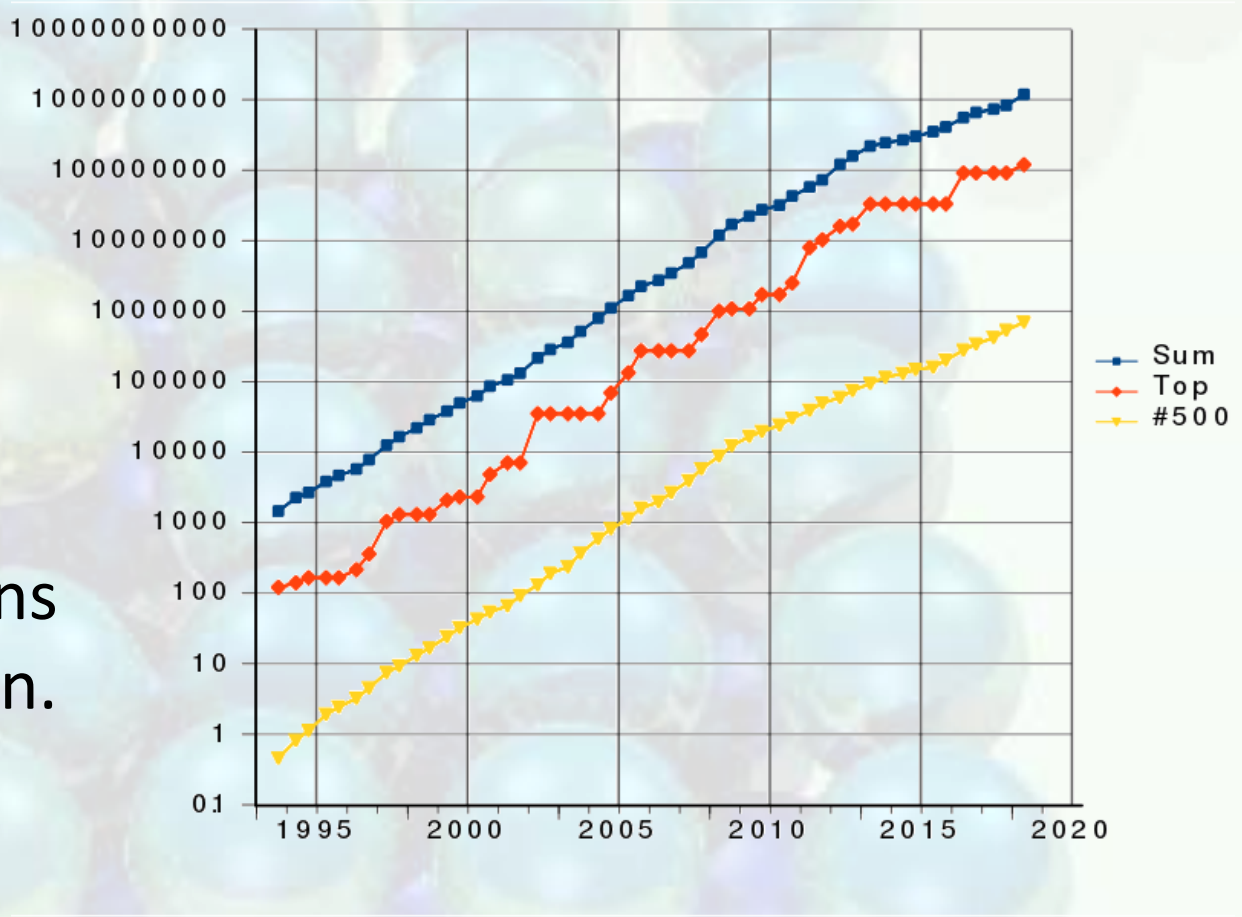
FEEDING 7 BILLION PEOPLE

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.



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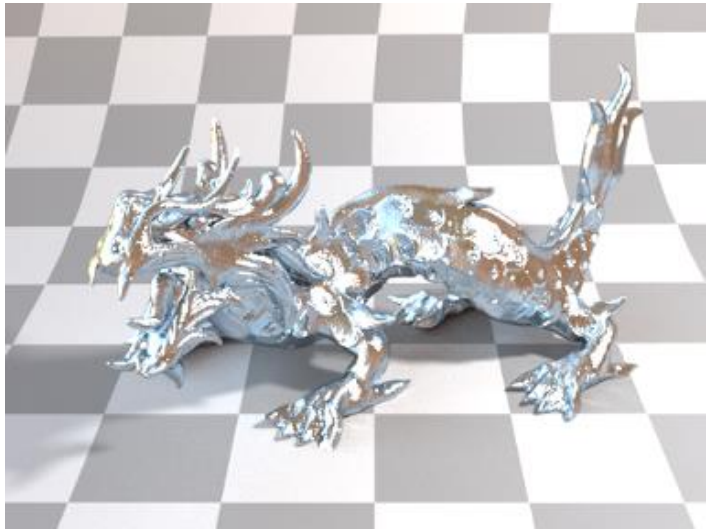
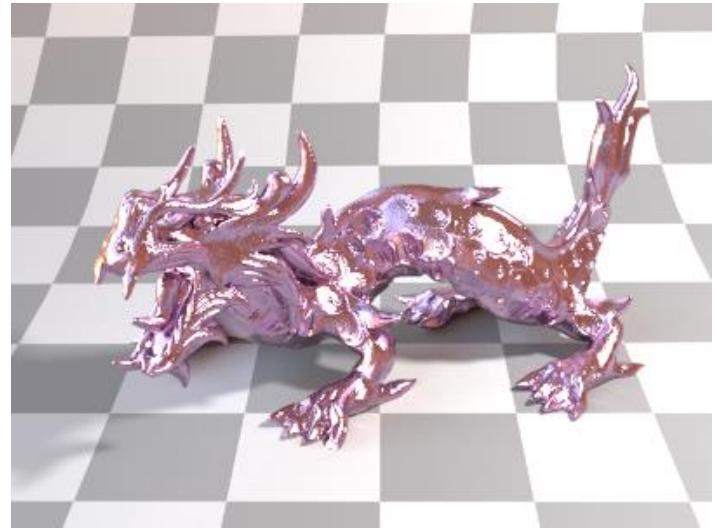
HOW WELL CAN WE REPRODUCE THE REAL WORLD?





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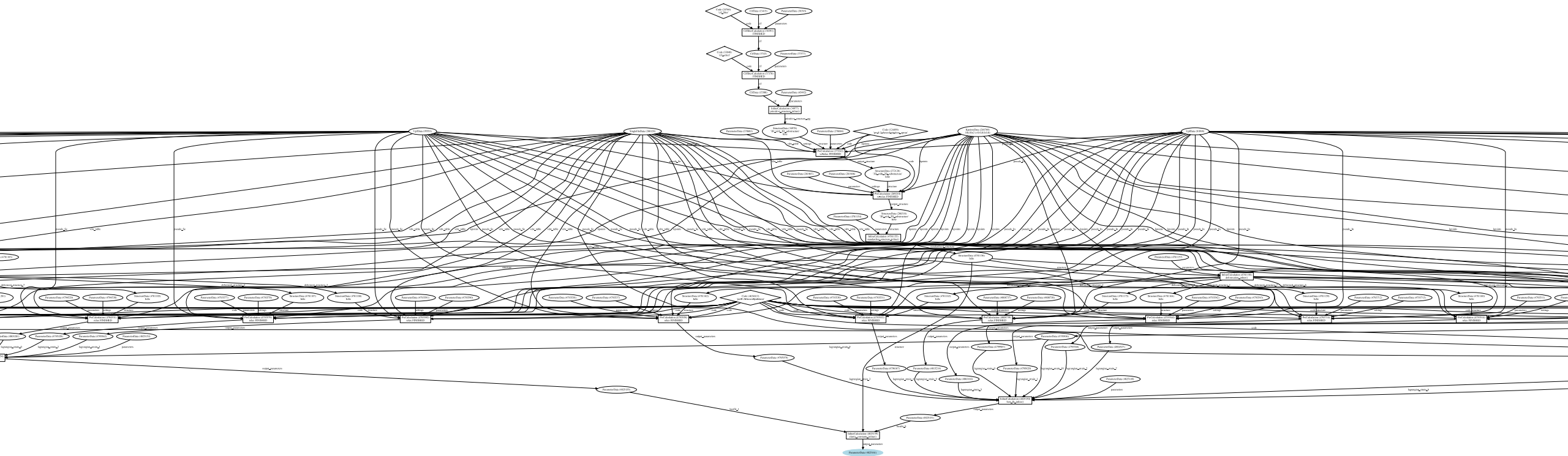
AUTOMATED, HIGH-THROUGHPUT, ON-DEMAND DATA

Input: Structure



Output: Property

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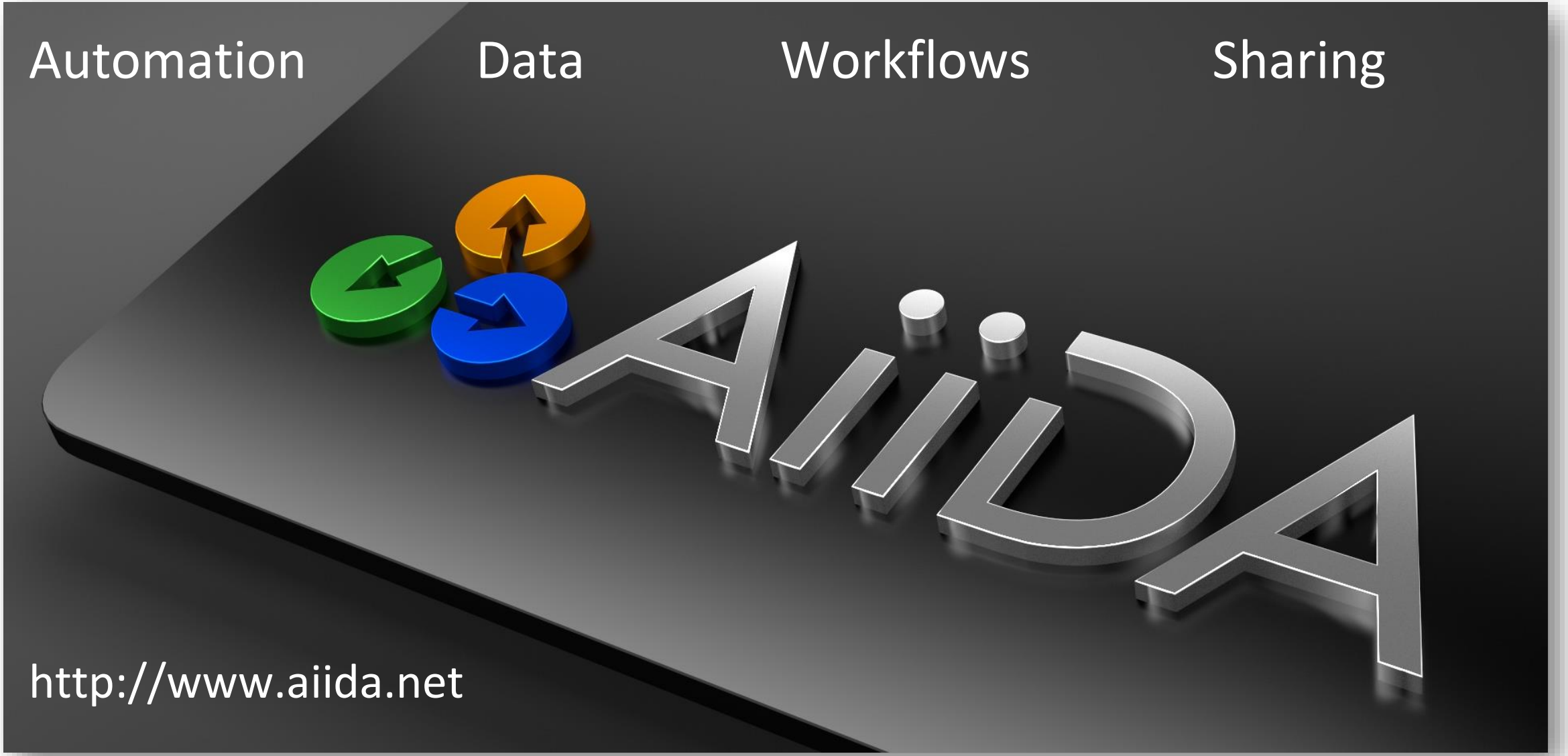
WE BUILT AN ENTIRE OPERATING SYSTEM FOR THIS



MACHINE LEARNING: FROM ONE MONTH TO ONE MINUTE

NEWS FEATURE

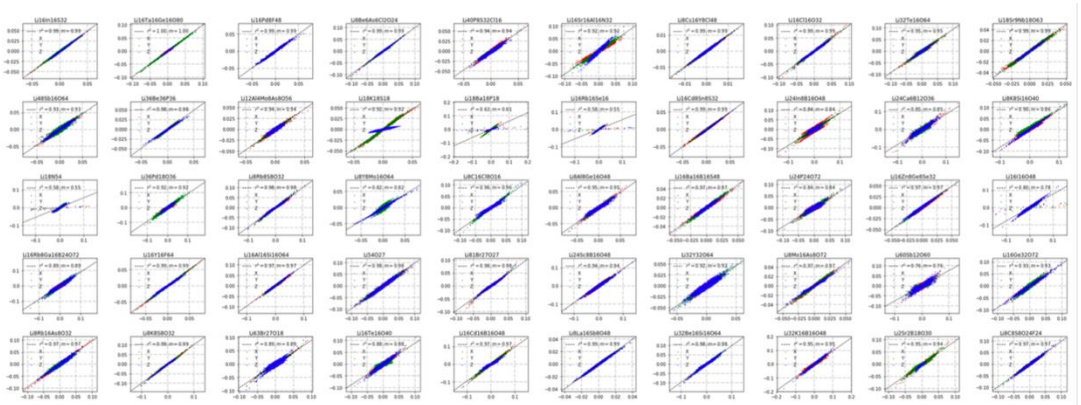
THE MATERIAL CODE

Machine-learning techniques could revolutionize how materials science is done.

BY NICOLA NOSENGO

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!"



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DEVELOPING SAFE, MORE POWERFUL BATTERIES

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

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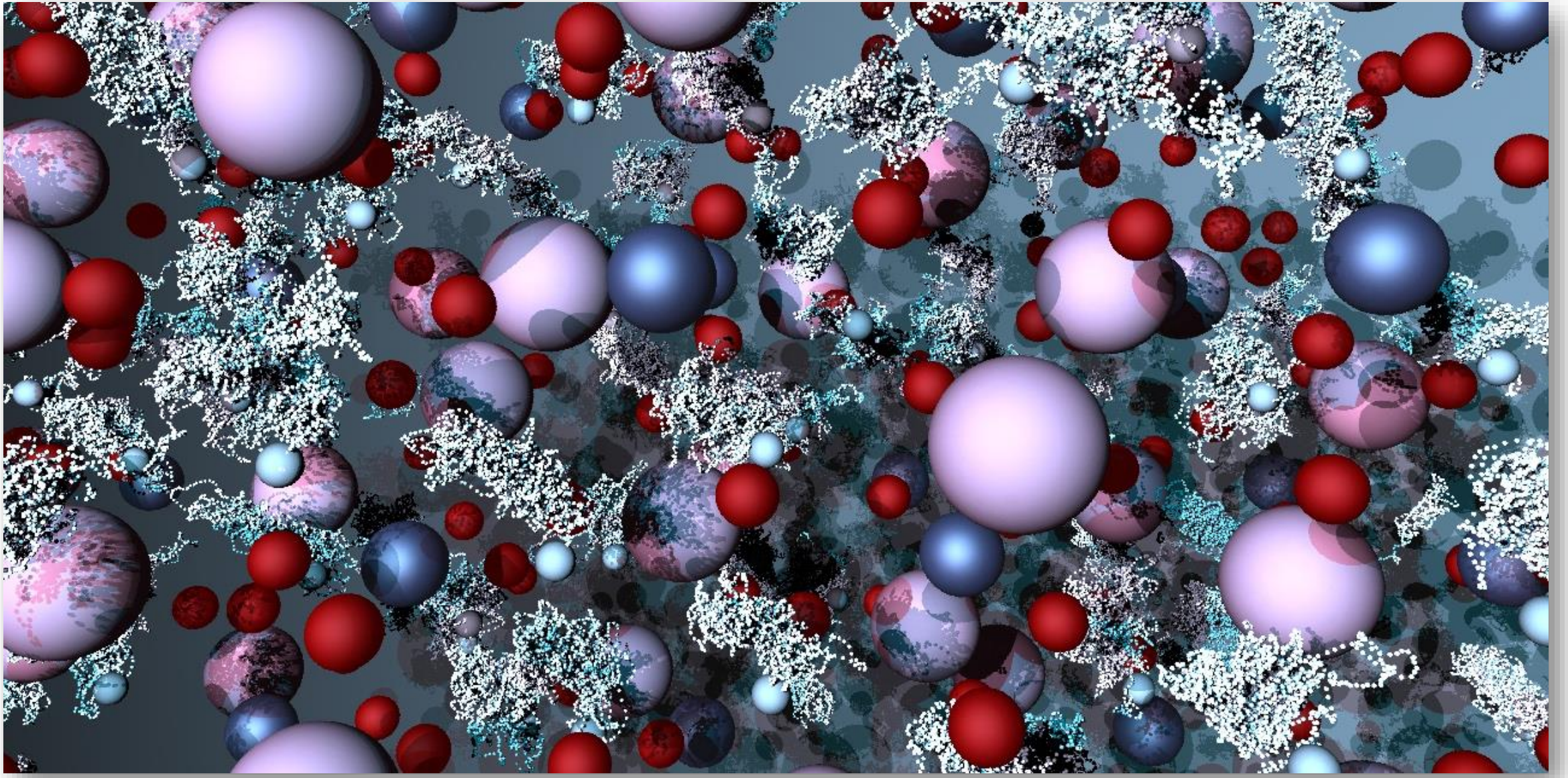
NEW SOLID STATE CONDUCTORS



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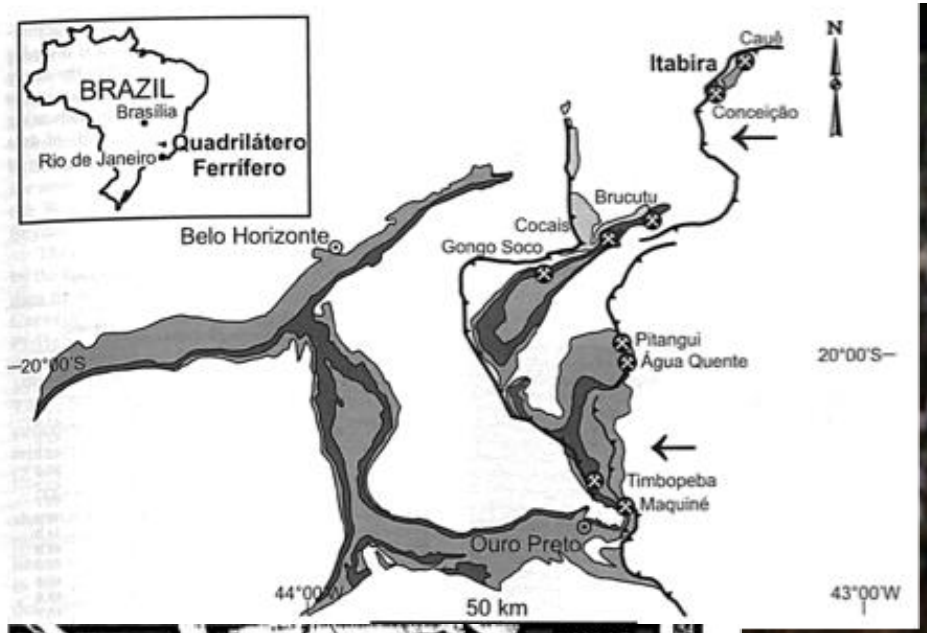
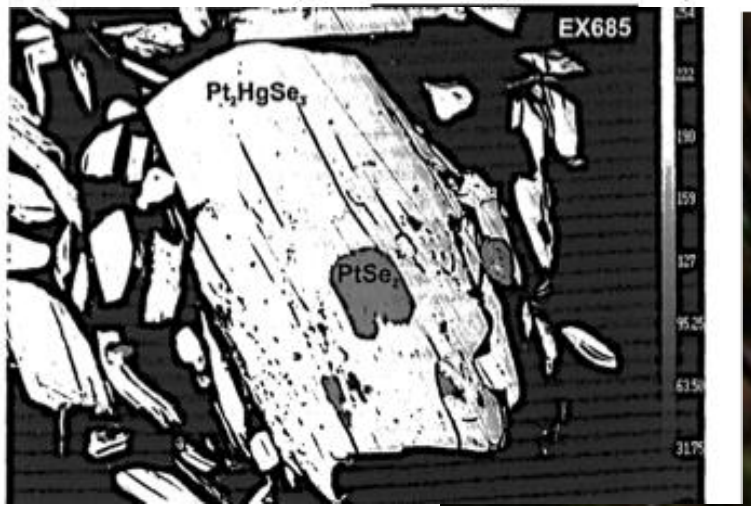
A ROOM-TEMPERATURE TOPOLOGICAL INSULATOR





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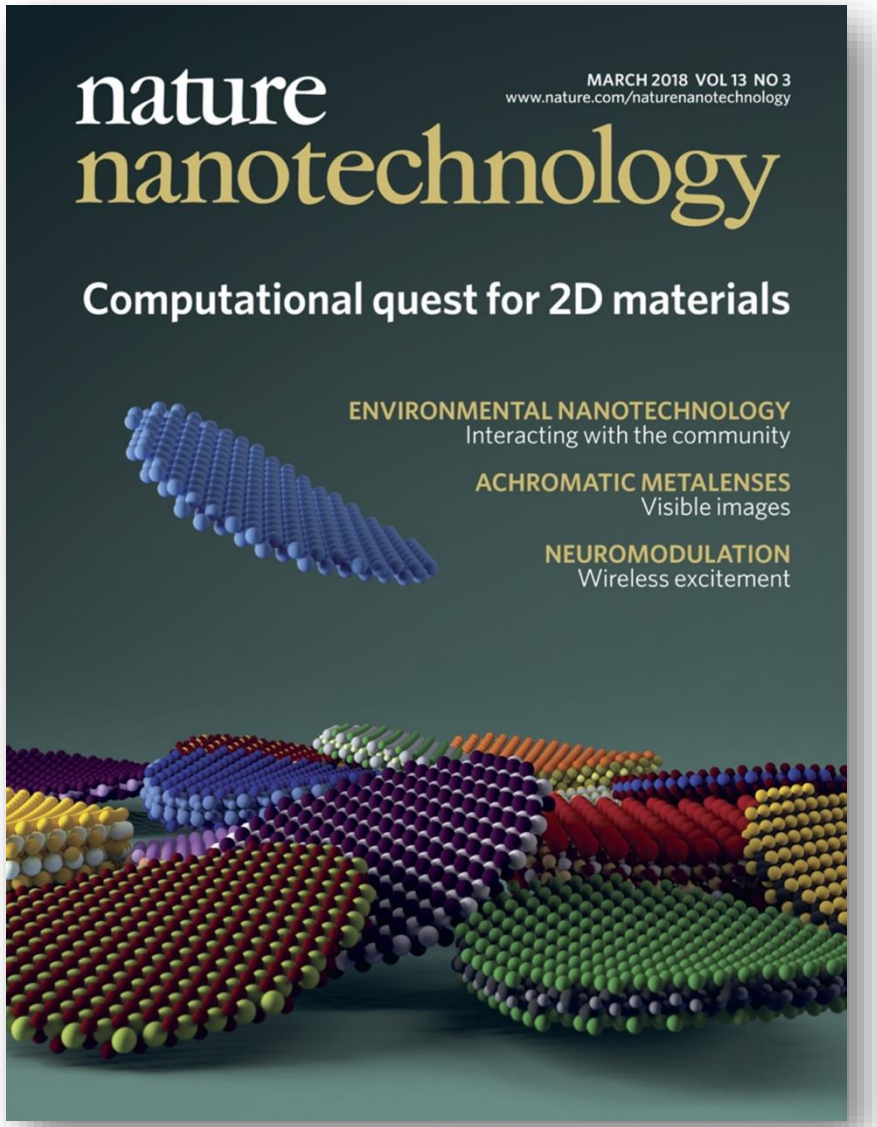
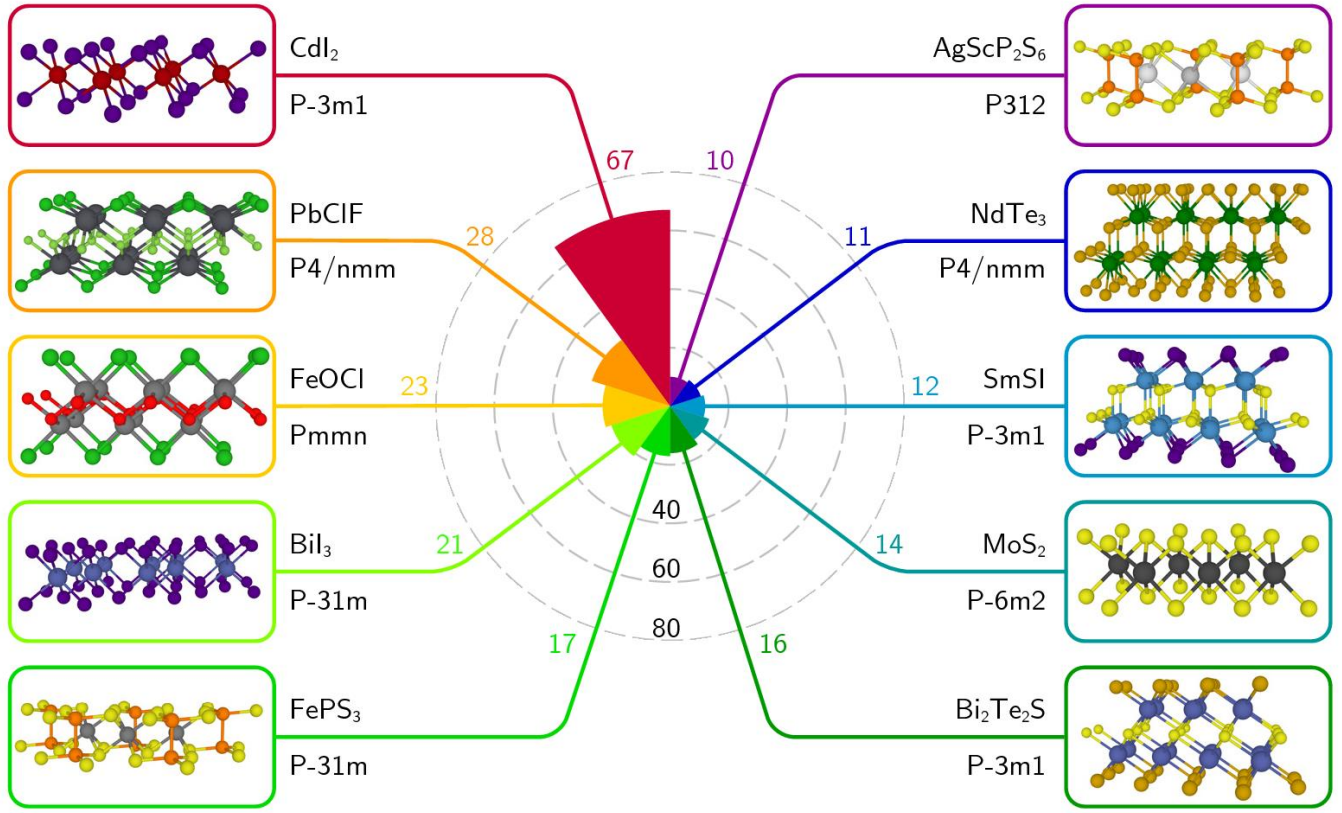
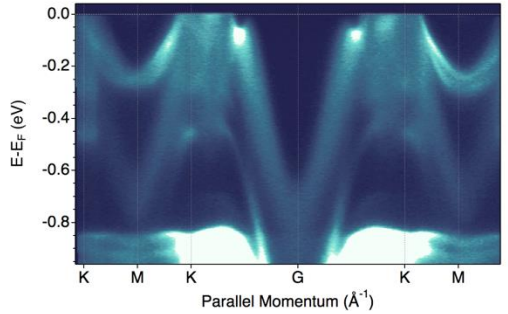
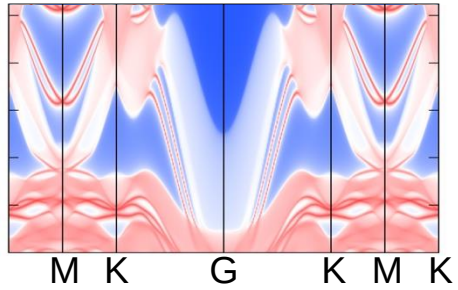
2000 NOVEL TWO DIMENSIONAL MATERIALS









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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