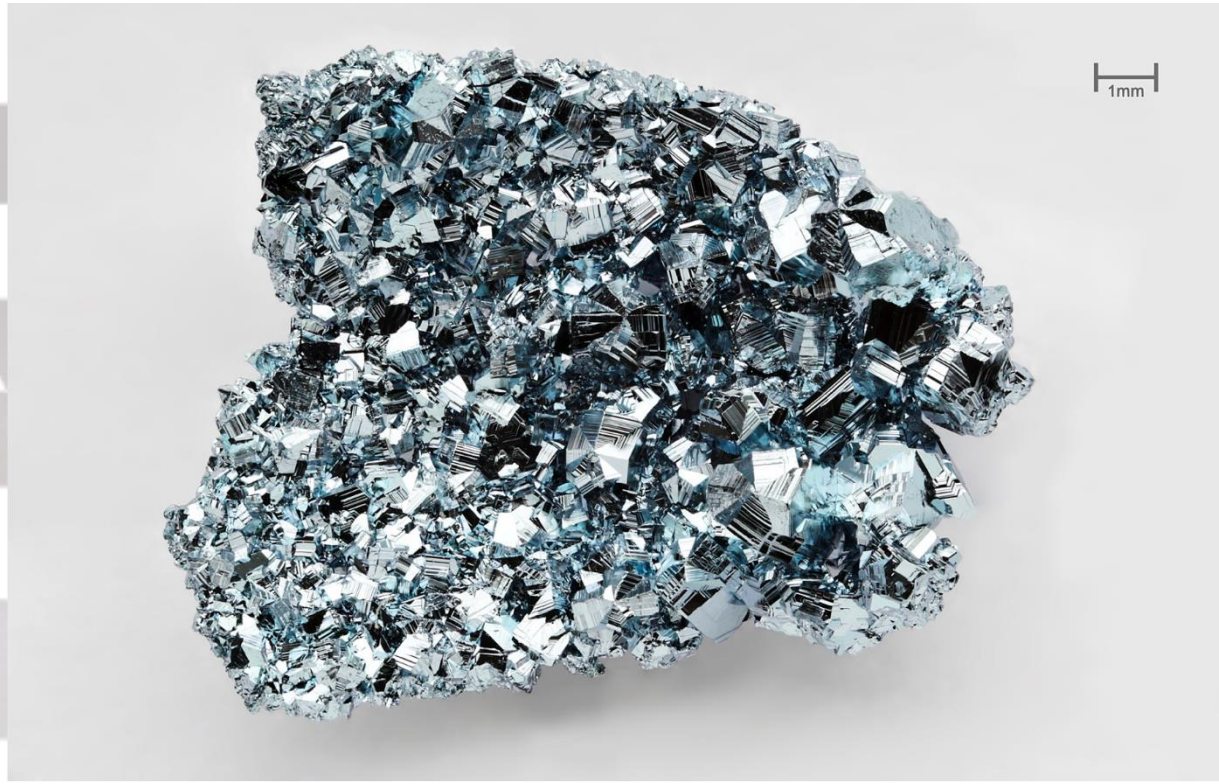
A GOLDEN AGE FOR MATERIALS SIMULATIONS

NICOLA MARZARI

THEORY AND SIMULATION OF MATERIALS, EPFL
CENTER FOR SCIENTIFIC COMPUTING, THEORY, AND DATA, PSI



TWO TAKE HOME MESSAGES

1) Materials enable the technologies that drive our economy and transform our world and our societies.

TWO TAKE HOME MESSAGES

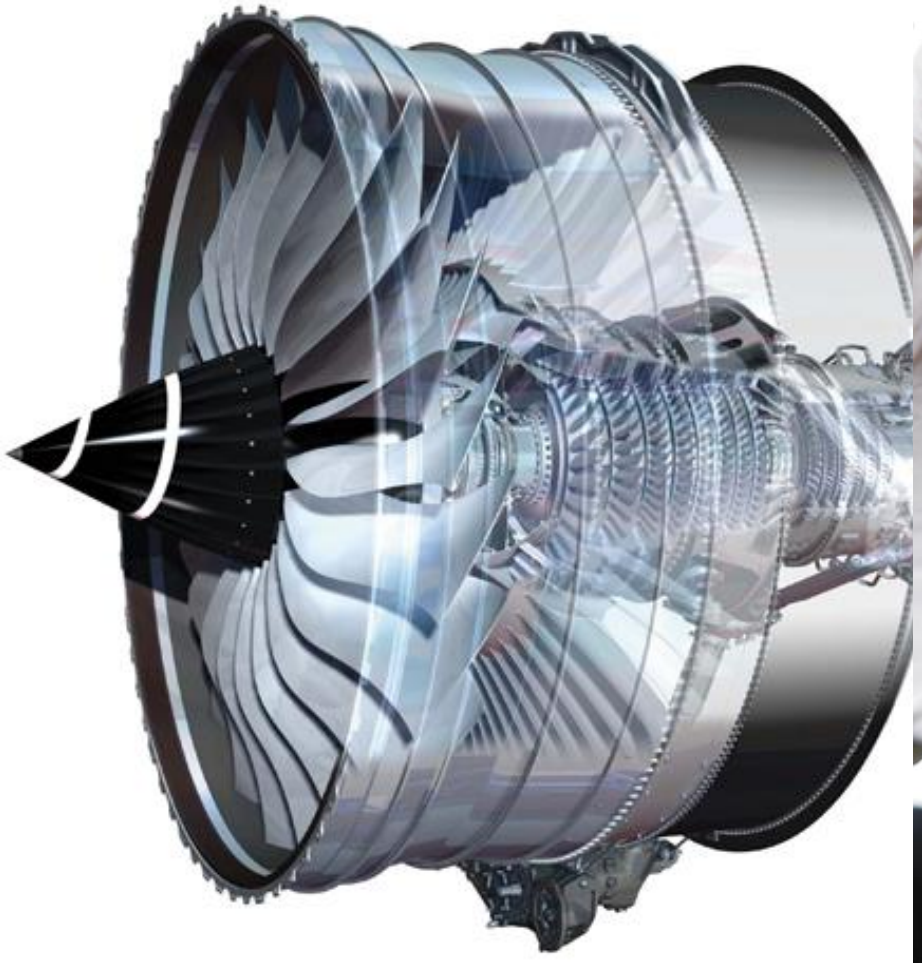
1) Materials enable the technologies that drive our economy and transform our world and our societies.

2) Theoretical and algorithmic advances, computational power, ML, and AI are changing our entire paradigm of scientific discovery and technological innovation.

HOW DO MATERIALS TRANSFORM SOCIETIES?

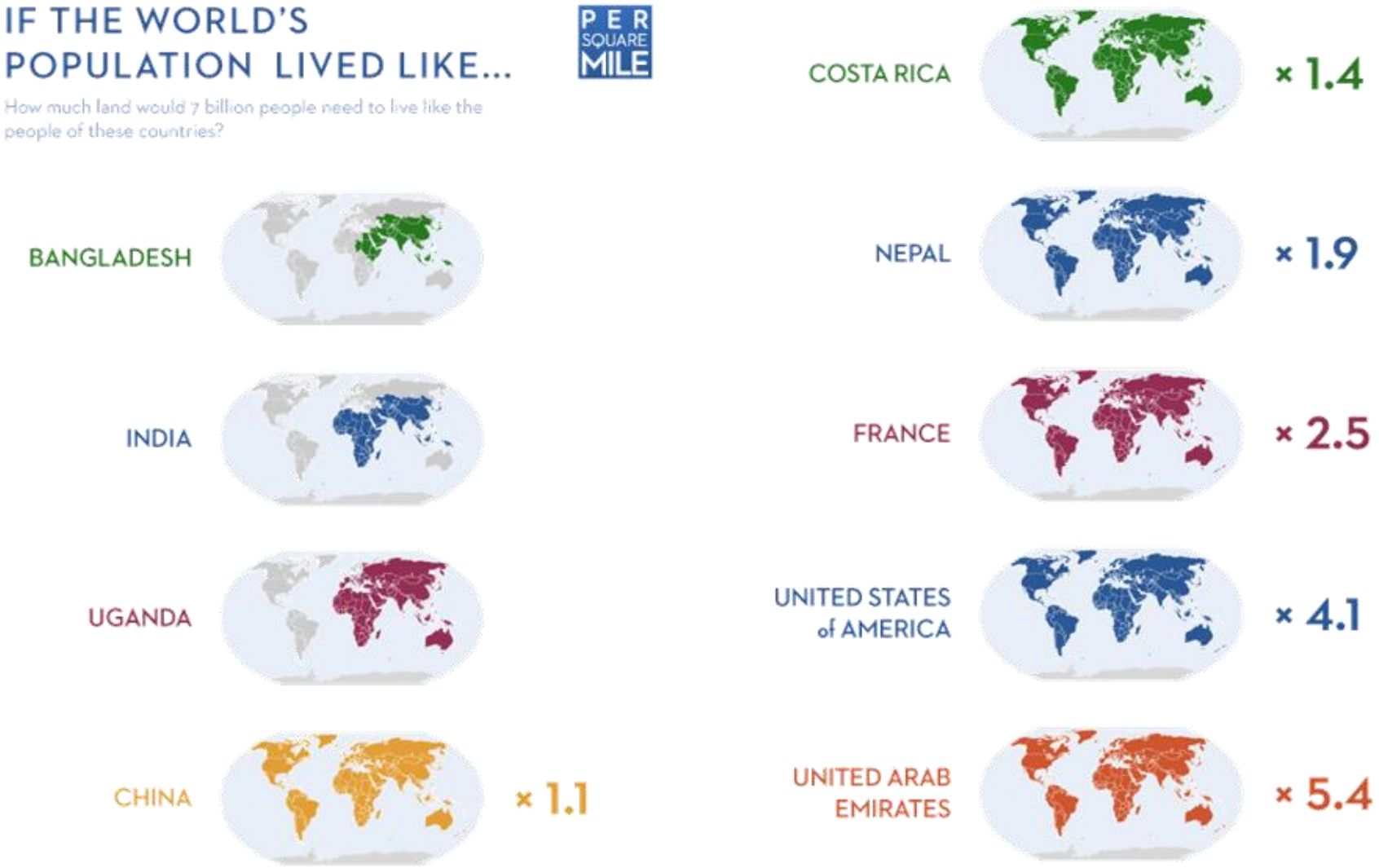
CLARA AND FRITZ

NEXT TIME YOU FLY

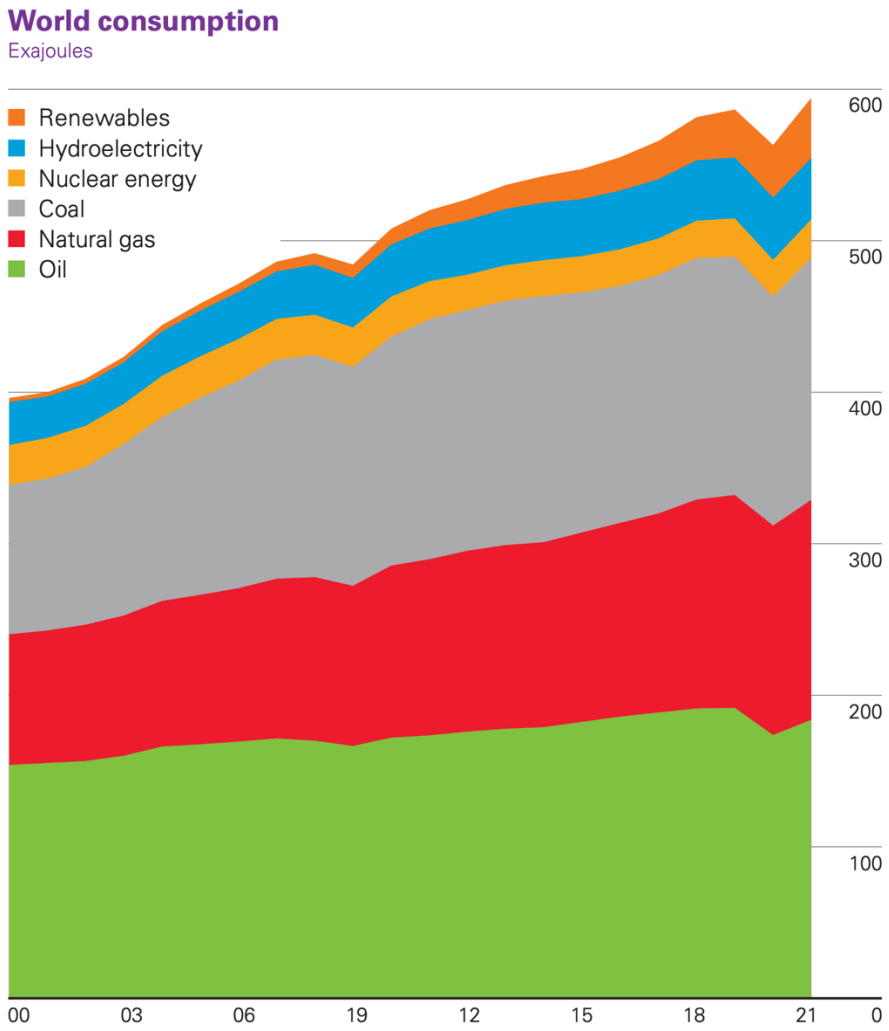


@Rolls-Royce

HUMAN FOOTPRINT (ERICH WIMMER: NO PLANET B!)



WORLD ENERGY CONSUMPTION (in Exajoules)



Renewables

Hydro

Nuclear

Coal

Natural gas

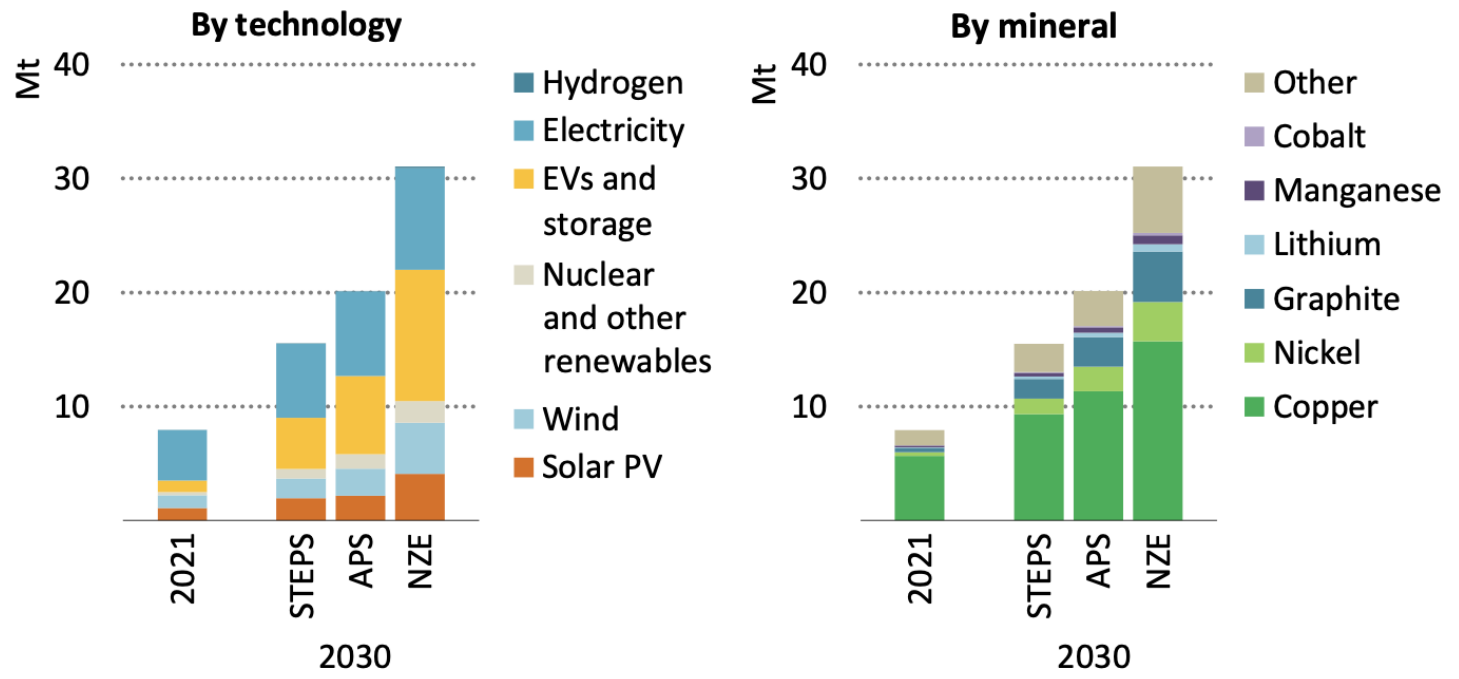
Oil

600 Exajoules/year =
100 billion barrels/year =
12 barrels/person/year

@BP Statistical Review of World Energy 2022

DIRTY MINERALS FOR CLEAN ENERGY

Figure 1.11 ▷ Mineral requirements for clean energy technologies by scenario, 2021 and 2030



Mineral requirements for clean energy technologies quadruple to 2030 in the NZE Scenario, with particularly high growth for materials for electric vehicles

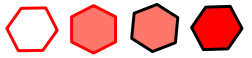
International Energy Agency | World Energy Outlook 2022

MARVEL VISION – 2011/12

1) **Accelerated design and discovery of materials** displaying novel physics or improved properties via a
2) materials' informatics platform of **database-driven, high-throughput** quantum simulations
3) **predictive accuracy** supported by advanced or innovative electronic-structure capabilities,
4) **verified and validated** thanks to code interoperability and automated benchmarking
5) **applied to materials** for energy, information-and-communication technologies, and pharmaceuticals.

MARVEL VISION – 2011/12

1) **the writers:** a community of **database-driven interoperable quantum engines**
2) **the library:** a **database of materials**, of materials' properties and performance, and of the results of quantum simulations, that starts with the structures of known materials, and that continuously expands
3) **the language:** a **data management system** that allows to store data heterogeneously, in its original and usually most natural format
4) **the librarian:** **the agent** that controls the quantum engines, reads the library, directs the effort to fill the library with the missing pieces, and addresses the grand challenges of the vertical materials design projects



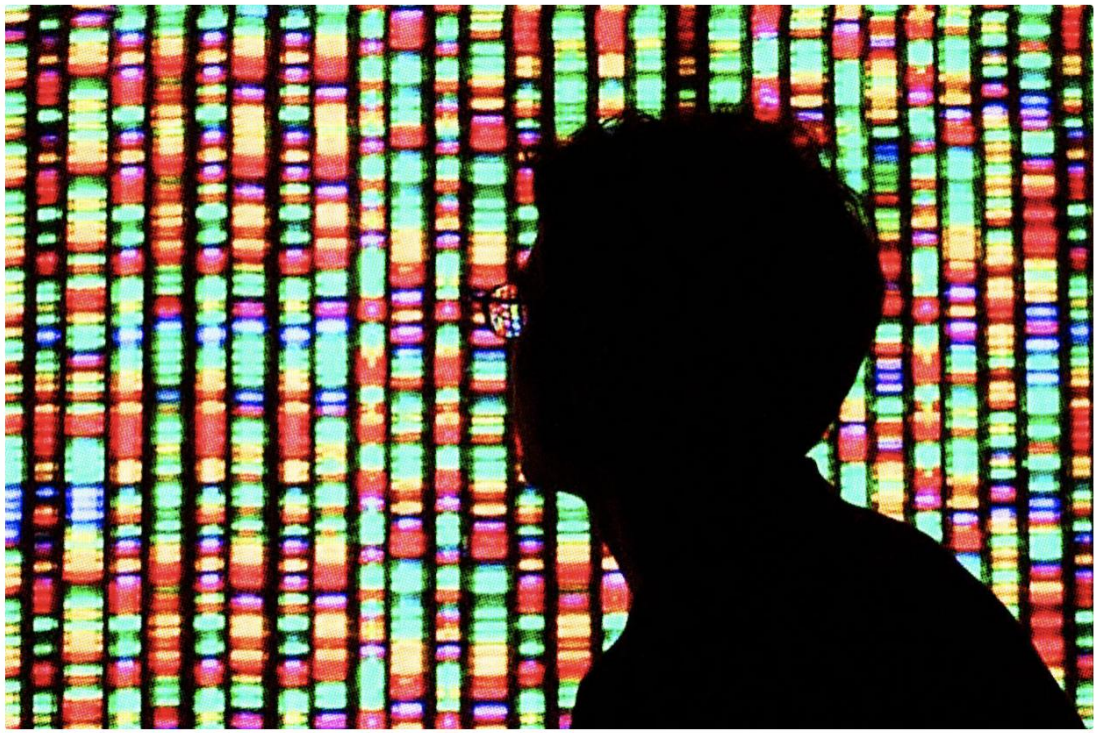
ADDRESS KEY ISSUES FOR SOCIETAL WELL BEING

- Energy harvesting, conversion, storage, efficiency
- Environmental protection and reparation
- High-tech and high-value industries
- Health care and biomedical engineering
- Pharmaceuticals
- Monitoring, provenance, and safety of foods
- Information and communication technologies
- Fundamental science (from 2D materials to entangled spins)
- Experimental science (detectors and sensors)

MATERIALS REVOLUTION

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

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



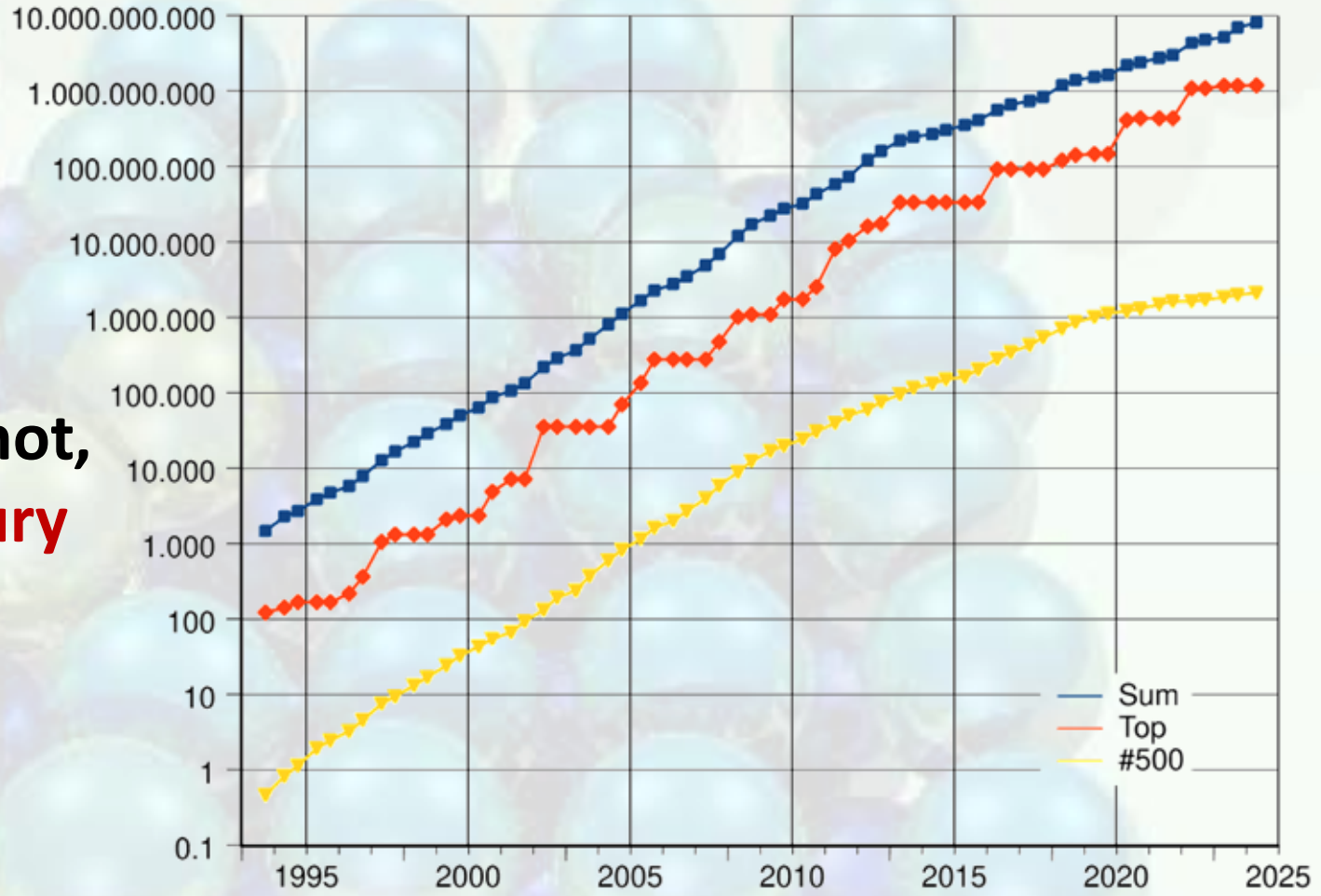
Yet today, we're in the midst of a materials revolution. Powerful simulation techniques, combined with increased computing power and machine learning, are enabling researchers to automate much of the discovery process, vastly accelerating the development of new materials

BARRON'S (April 2019)

THE BUSINESS MODEL: 100% RETURNS EVERY 16-18 MONTHS

A calculation that took one year in 1993 takes one second in 2026 (30-million-fold increase).

Just with bits. **Qubits maybe not, ML and AI for sure. 21st-century science and technology will greatly benefit from, and be driven by, computational science.**



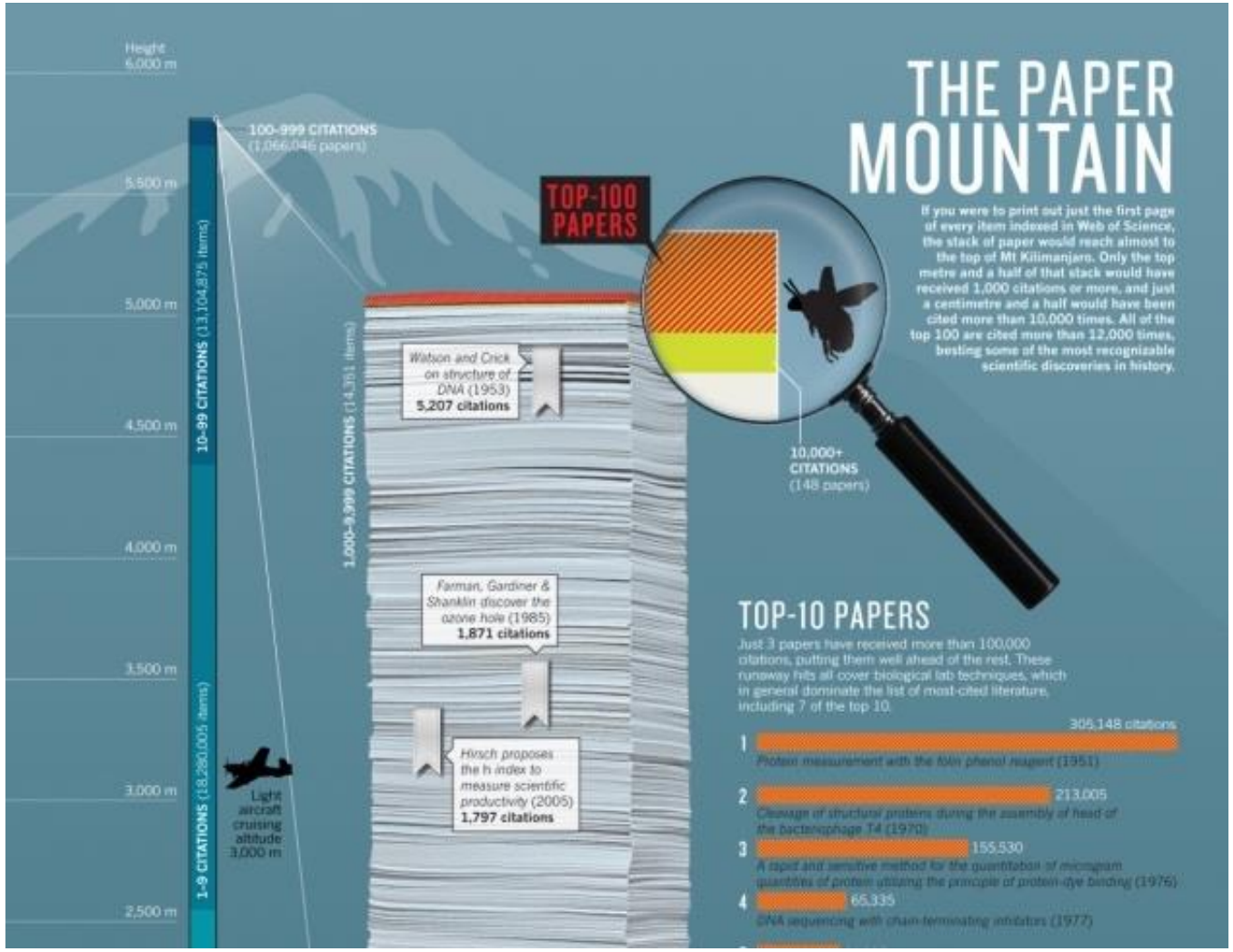
IMPACT OF FIRST-PRINCIPLES SIMULATIONS

THE TOP 100 PAPERS:

12 papers on electronic-structure simulations in the top-100 most cited papers in the entire scientific-medical-engineering literature.

2 in the top 10

NATURE, OCT 2014



IMPACT OF FIRST-PRINCIPLES SIMULATIONS

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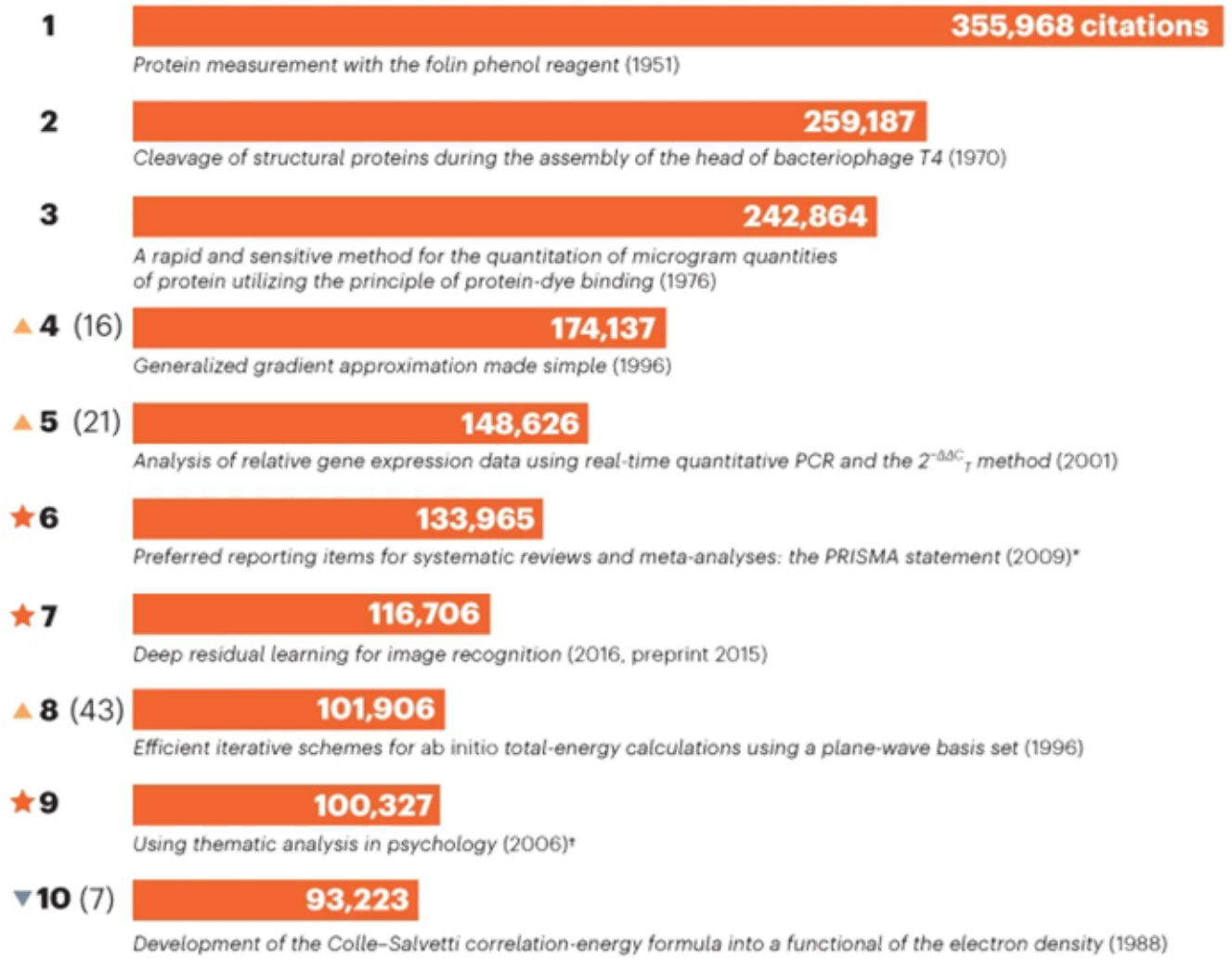
3 in the top 10

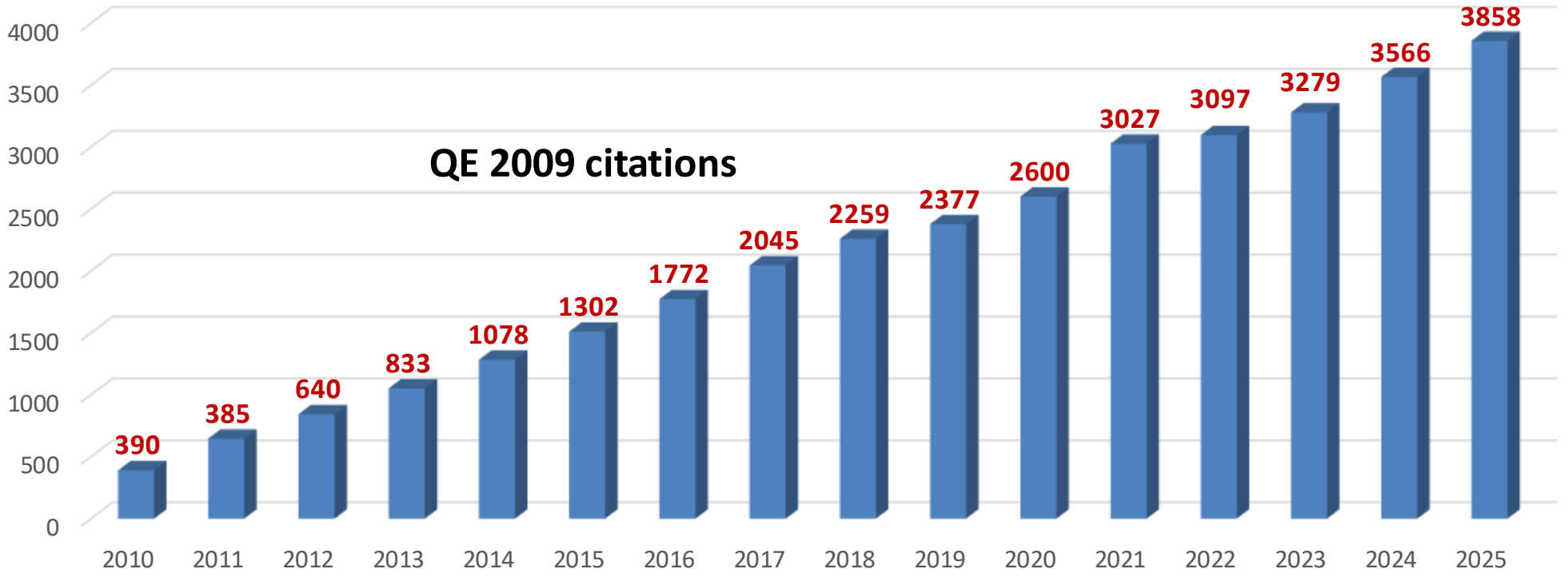
NATURE, APR 2025



THIS IS BIG SCIENCE

CERN: 1086 papers in 2025; 2026 budget: 1.65 bn EUR

Quantum ESPRESSO: 3858+ papers in 2025; 2026 budget: 🥜🥜🥜 EUR



THE ANSWER IS 42 (YEARS)

VOLUME 26, NUMBER 8

Pseudopotentials that work: From H to Pu

G. B. Bachelet,* D. R. Hamann, and M. Schlüter
Bell Laboratories, Murray Hill, New Jersey 07974
(Received 28 April 1982)

nature reviews physics
https://doi.org/10.1038/s42254-023-00655-3

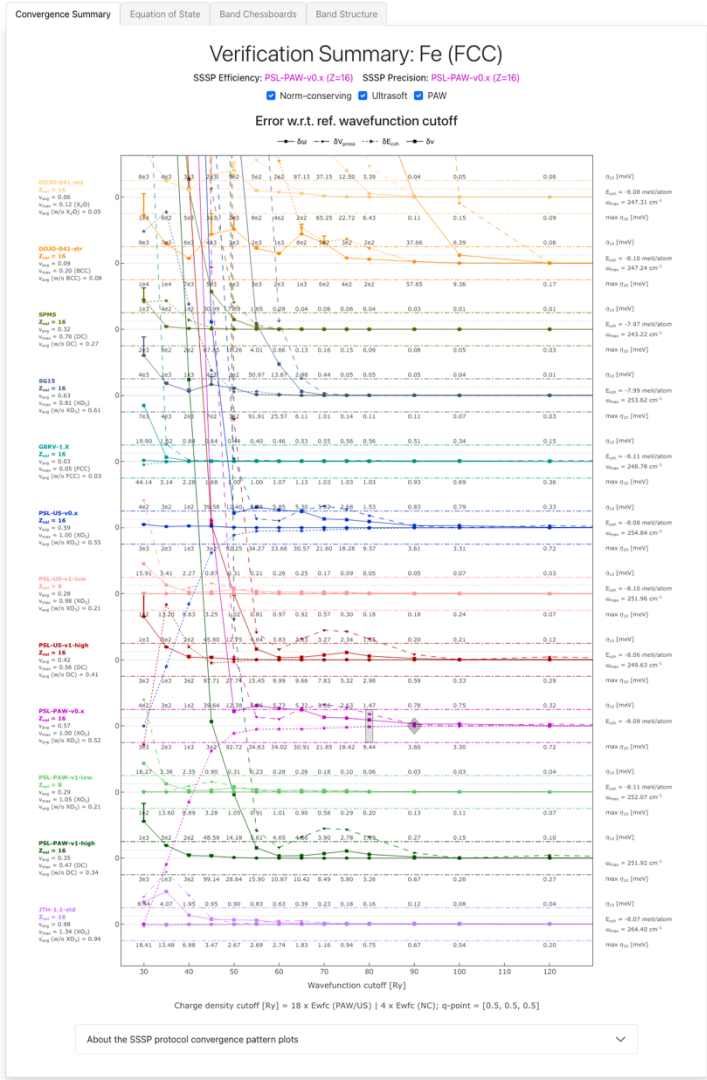
Expert recommendation

Check for updates

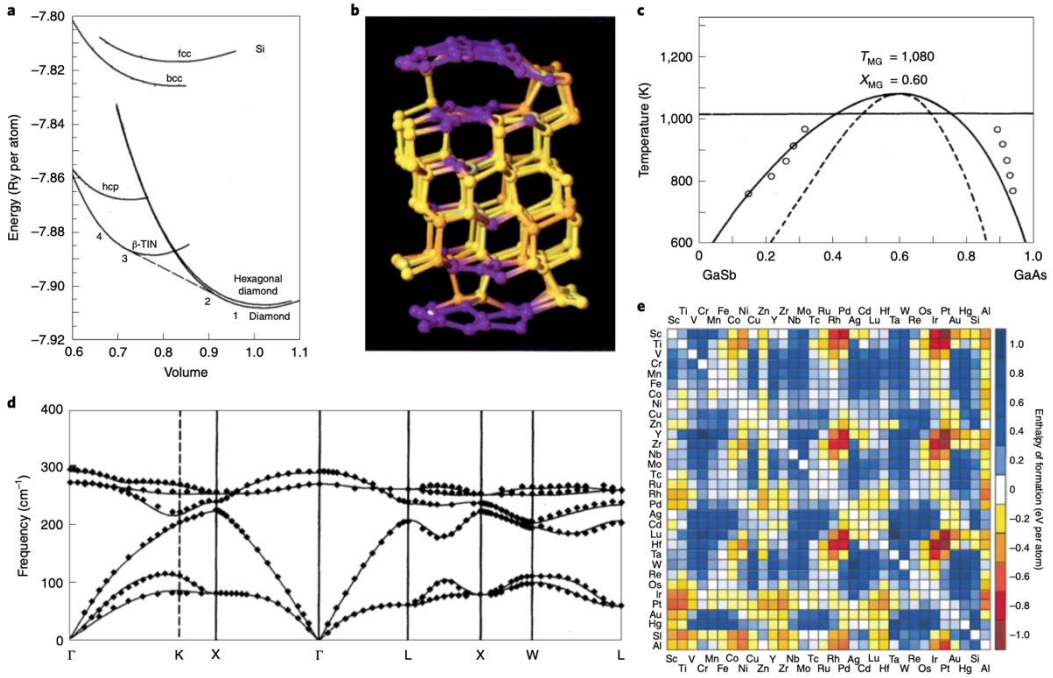
How to verify the precision of density-functional-theory implementations via reproducible and universal workflows

Emanuele Bosoni[1], Louis Beal[2], Marnik Bercx[3], Peter Blaha[4], Stefan Blügel[5], Jens Bröder[5,6], Martin Callsen[7,8,9], Stefaan Cottenier[7,8], Augustin Degomme[2], Vladimir Dikan[1], Kristjan Eimre[3], Espen Flage-Larsen[10,11], Marco Fornari[12], Alberto Garcia[1], Luigi Genovese[2], Matteo Giantomassi[13], Sebastiaan P. Huber[3,14], Henning Janssen[5], Georg Kastlunger[15], Matthias Krack[16], Georg Kresse[17,18], Thomas D. Kühne[19,20], Kurt Lejaeghere[8,21], Georg K. H. Madsen[4], Martijn Marsman[17,18], Nicola Marzari[3,16], Gregor Michalicek[5], Hossein Mirhosseini[22], Tiziano M. A. Müller[23], Guido Petretto[13], Chris J. Pickard[24,25], Samuel Poncé[13], Gian-Marco Rignanese[13], Oleg Rubel[26], Thomas Ruh[4,8,27], Michael Sluydts[7,8,28], Danny E. P. Vanpoucke[7,29], Sudarshan Vijay[15], Michael Wolloch[17,18], Daniel Wortmann[5], Aliaksandr V. Yakutovich[30], Jusong Yu[3,16], Austin Zadoks[3], Bonan Zhu[31,32] & Giovanni Pizzi[3,16]

https://sssp.materialscloud.org



WHAT CAN WE DO?



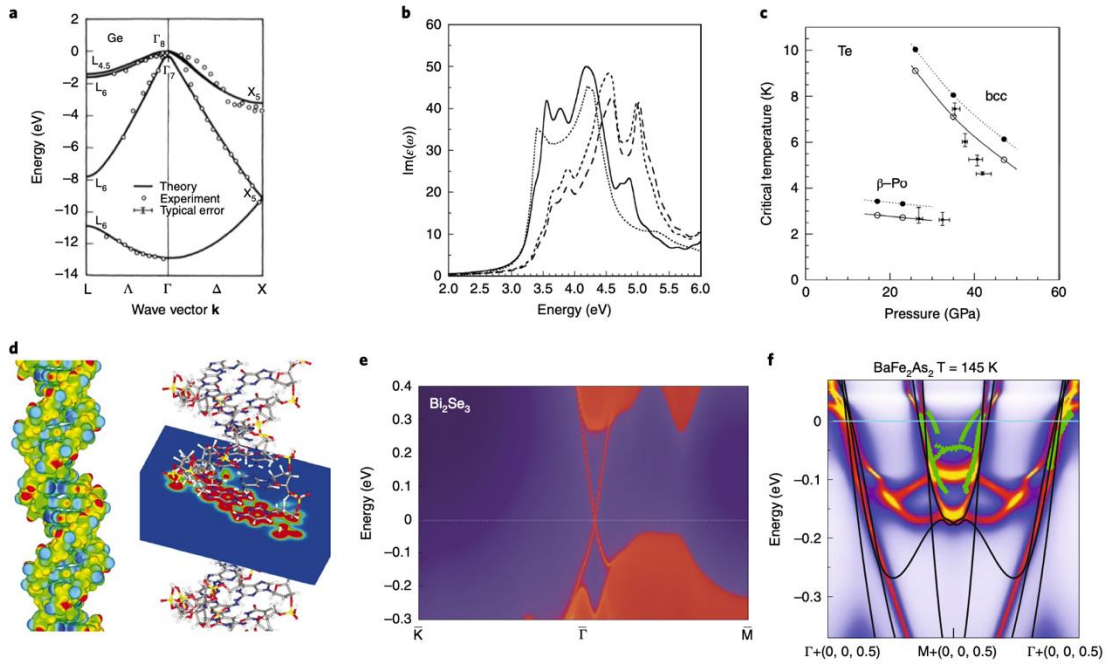
N. Marzari, A. Ferretti, and C. Wolverton, Nature Materials 20, 736–749 (2021)

Table 1 | An overview of selected materials properties that can be obtained from DFT ground-state calculations

Materials properties	Models and theories	Electronic-structure toolbox
Atomic and cell geometries at fixed volume or pressure[13,166]	Hellmann–Feynman theorem	Total energy, forces and stresses
Zero-temperature stability[141–143]: formation energies, elastic constants, defects concentrations[167]	Equations of state (Murnaghan, Birch, …), convex hulls, self-consistent chemical potentials	Total energies, forces and stresses for all different phases, defects, periodic-boundary corrections for charged defects
Chemistry and reactivity[84,85], surface science[88]	Potential-energy surfaces, transition-state theory, volcano plots, kinetic Monte Carlo, rate equations, conical intersections, Marcus theory, Franck–Condon principle	Total energies and forces, van der Waals functionals, nudged-elastic-band method, constrained DFT, non-adiabatic dynamics (surface hopping, Ehrenfest)
Phonon dispersions and thermomechanical properties[18], thermal and electrical transport[19], superconductivity[168]	Linear-response theory, quasi-harmonic approximation, Grüneisen parameters, Boltzmann transport equation, equilibrium/non-equilibrium Green's functions, Allen–Dynes formula, Migdal–Eliashberg equations, superconducting DFT	Density functional perturbation theory and $2n+1$ theorem for el–ph, ph–ph interactions, Born effective charges, dielectric tensor
Dielectric[18], magnetic[123] and topological properties[125], ferroelectrics[92] and multiferroics[169]	Linear-response theory, modern theory of polarization and of magnetization, electric enthalpy, model Hamiltonians, topological invariants	Berry phases, maximally localized Wannier functions, Wilson loops, spin–orbit coupling
Magnetic phases[54], magnetic anisotropy, spin waves[55], skyrmions[56]	Spin Hamiltonians (Ising, Heisenberg, Dzyaloshinskii–Moriya), paramagnetism as ensemble average	Spin–orbit coupling, non-collinear magnetism, force theorem, spin-density functionals
Thermodynamic ensembles[71,77,78]: finite-temperature properties and Helmholtz or Gibbs free energies[81], transport coefficients[108]	Molecular dynamics, Monte Carlo, thermodynamic integration, metadynamics, path-integral molecular dynamics, Green–Kubo relations	Born–Oppenheimer and Car–Parrinello molecular dynamics, density functional perturbation theory, thermostats and barostats, ring-polymer mapping
Thermodynamic ensembles[88,129,130,170]: composition, chemical potential, partial pressure	Lattice Hamiltonians, Monte Carlo, mean-field approximation, cluster variation method, model entropies, special quasirandom structures	Cluster expansions, computational alchemy
Electrochemistry[86,89], pH[90], operando studies	Grand-canonical simulations for electrons and ions, embedding, double-layer and diffuse-layer models	Computational hydrogen electrode, model solvents and electrolytes, Poisson–Boltzmann solvers, ensemble simulations, coupling with reservoirs
Macroscopic mechanical properties[109,110] (strength, fracture, and plasticity), soft matter, biomolecules	Multiscale simulations, QM-MM, dislocation dynamics, effective volumes	Force fitting, learn-on-the-fly, neural networks and kernel-regression potentials
Microscopies[171]: STM, AFM, TEM	Tersoff–Hamann model, electron scattering	Local density of states, first-principles molecular dynamics, all-electron charge density and potential, PAW reconstructions

If the exact functional were known, these properties would be exactly reproduced, provided all the microscopic phenomenology were included. The second column points to the broader concepts, models and phenomenology from physics, chemistry and materials science; the third column highlights the electronic-structure quantities, algorithms and theories that are typically coded. Band-structure properties require more advanced methods, but are often approximated using KS states. STM, scanning tunnelling microscopy; AFM, atomic force microscopy; TEM, transmission electron microscopy; QM-MM, quantum mechanics - molecular mechanics; el, electron; ph, phonon; PAW, projector augmented wave.

WHAT CAN WE DO?



N. Marzari, A. Ferretti, and C. Wolverton, Nature Materials 20, 736–749 (2021)

Table 2 | A selected overview of spectroscopic properties that can be obtained from DFT ground-state calculations or from excited-state spectral formulations

Spectroscopic properties	Models and theories	Electronic-structure toolbox
Vibrational spectroscopies[18,19]: infrared, Raman and hyper-Raman, SERS, SEIRAS, and SFG, IETS, HREELS, INS	Vibrations from harmonic and adiabatic approximations, anhamonicity, Placzek and Albrecht approximation, Fermi golden rule	Phonon frequencies, dispersions and lifetimes, electron–phonon matrix elements. Born effective charges, frequency-dependent electric tensor, polarizability tensor, electric enthalpy, electric-field gradients
'Charged excitation' spectroscopies[66,114]: direct and inverse photoemission, ARPES[61], UPS, STS[171]	Quantum field theory of electron–electron and electron–boson interactions, diagrammatic perturbation theory, Hedin's equations, one-step and three-step models, Tersoff–Hamann model	Green's functions and self-energies, GW approximation, vertex corrections, cumulants, electron–phonon self-energies, DMFT, Koopmans spectral functionals, hybrids/range-separated/dielectric-dependent functionals
'Neutral excitation' spectroscopies[66]: optical absorption and luminescence[172,173], Stokes shifts, colour and reflectivity[174], nonlinear optics and second harmonic generation[175], (non-resonant) IXS, EELS, resonant Raman, Auger recombination[176]	Light–matter interaction, electron scattering, linear and nonlinear response, first- and second-order Fermi golden rules, excited-state relaxations, trichromatic theory, Kramers–Heisenberg	TDDFT, Casida equations, Bethe–Salpeter equation, optical ($\mathbf{q}=0$) and finite-$\mathbf{q}$ limits of the dielectric response, real-time propagation
Magnetic spectroscopies[113]: NMR, EPR, quadrupolar coupling, g-tensor, hyperfine couplings, Knight shifts, MCD, muon spin spectroscopy, magnons[55]	Effective nuclear Hamiltonians, linear-response theory, modern theory of magnetization	Gauge-including projector augmented waves, Berry phases and converse NMR, all-electron reconstruction, electric-field gradients, TDDFT
X-ray spectroscopies: XPS[114], XAS[177,178] (XANES, EXAFS), RIXS, Compton scattering, XMCD	Light–matter interaction, Fermi golden rule, crystal-field splitting, multiplets and model Hamiltonians, dipole and impulse approximations	Full and half core-hole pseudopotentials, total energies, electronic states from DFT, GW, Bethe–Salpeter and wavefunction methods
Real-time[64,65,179], ultrafast, pump–probe[62,63,106] and two-dimensional spectroscopies	Out-of-equilibrium dynamics, time-dependent Boltzmann transport, Keldysh non-equilibrium Green's function, Kadanoff–Baym equations	DFT, real-time propagation TDDFT, time-dependent current DFT, Ehrenfest dynamics, non-equilibrium Green's functions
Quantum optics[67,180,181]	Field quantization	QED DFT, QED many-body perturbation theory

See also Table 1 footnote. SERS, surface-enhanced Raman spectroscopy; SEIRAS, surface-enhanced infrared absorption spectroscopy; SFG, sum-frequency generation; IETS, inelastic electron tunnelling spectroscopy; HREELS, high-resolution electron energy loss spectroscopy; INS, inelastic neutron scattering; ARPES, angle-resolved photoemission spectroscopy; UPS, ultraviolet photoemission spectroscopy; STS, scanning tunnelling spectroscopy; IXS, inelastic X-ray scattering; EELS, electron energy loss spectroscopy; NMR, nuclear magnetic resonance; EPR, electron paramagnetic resonance; MCD, magnetic circular dichroism; XPS, X-ray photoelectron spectroscopy; XAS, X-ray absorption spectroscopy; XANES, X-ray absorption near-edge structure; EXAFS, extended X-ray absorption fine structure; RIXS, resonant inelastic X-ray scattering; XMCD, X-ray magnetic circular dichroism; QED, quantum electrodynamics; **q**, quasi-momentum transfer.

MAJOR INVESTMENTS: FROM MAJOR COMPANIES…

Microsoft

Google DeepMind

MatterGen: Property-guided materials design

Published December 7, 2023

By Andrew Fowler, Senior Researcher; Matthew Horton, Senior Research SDE; Ryota Tomioka, Principal Research Manager; Robert Pinsler, Senior Researcher; Tian Xie, Principal Research Manager; Claudio Zeni, Senior Researcher; Daniel Zugner, Senior Researcher

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MatterSim: A deep-learning model for materials under real-world conditions

Published May 13, 2024

By Han Yang, Senior Researcher; Jielan Li, Researcher 2; Hongxia Hao, Senior Researcher; Ziheng Lu, Principal Researcher

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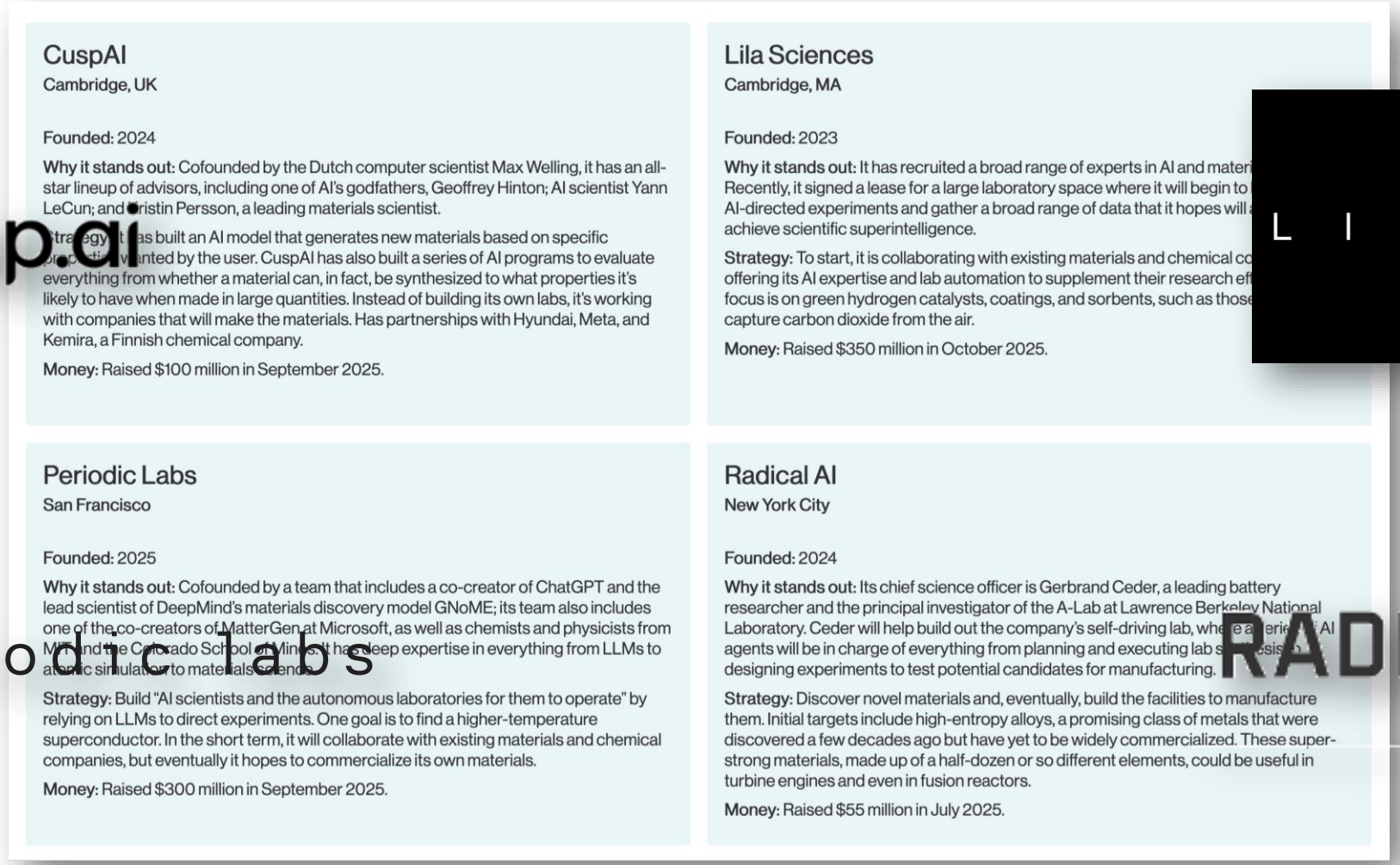
AI tool GNoME finds 2.2 million new crystals, including 380,000 stable materials that could power future technologies

Meta

Open Catalyst

AI at Meta and Carnegie Mellon University join forces to find more efficient and scalable ways to store and use renewable energy.

…TO 1B$ IN STARTUPS…



CuspAI
Cambridge, UK

Founded: 2024

Why it stands out: Cofounded by the Dutch computer scientist Max Welling, it has an all-star lineup of advisors, including one of AI's godfathers, Geoffrey Hinton; AI scientist Yann LeCun; and Kristin Persson, a leading materials scientist.

Strategy: It has built an AI model that generates new materials based on specific properties wanted by the user. CuspAI has also built a series of AI programs to evaluate everything from whether a material can, in fact, be synthesized to what properties it's likely to have when made in large quantities. Instead of building its own labs, it's working with companies that will make the materials. Has partnerships with Hyundai, Meta, and Kemira, a Finnish chemical company.

Money: Raised $100 million in September 2025.

Lila Sciences
Cambridge, MA

Founded: 2023

Why it stands out: It has recruited a broad range of experts in AI and materi… Recently, it signed a lease for a large laboratory space where it will begin to … AI-directed experiments and gather a broad range of data that it hopes will … achieve scientific superintelligence.

Strategy: To start, it is collaborating with existing materials and chemical co… offering its AI expertise and lab automation to supplement their research ef… focus is on green hydrogen catalysts, coatings, and sorbents, such as those … capture carbon dioxide from the air.

Money: Raised $350 million in October 2025.

Periodic Labs
San Francisco

Founded: 2025

Why it stands out: Cofounded by a team that includes a co-creator of ChatGPT and the lead scientist of DeepMind's materials discovery model GNoME; its team also includes one of the co-creators of MatterGen at Microsoft, as well as chemists and physicists from MIT and the Colorado School of Mines. It has deep expertise in everything from LLMs to atomic simulation to materials science.

Strategy: Build "AI scientists and the autonomous laboratories for them to operate" by relying on LLMs to direct experiments. One goal is to find a higher-temperature superconductor. In the short term, it will collaborate with existing materials and chemical companies, but eventually it hopes to commercialize its own materials.

Money: Raised $300 million in September 2025.

Radical AI
New York City

Founded: 2024

Why it stands out: Its chief science officer is Gerbrand Ceder, a leading battery researcher and the principal investigator of the A-Lab at Lawrence Berkeley National Laboratory. Ceder will help build out the company's self-driving lab, where AI agents will be in charge of everything from planning and executing lab … designing experiments to test potential candidates for manufacturing.

Strategy: Discover novel materials and, eventually, build the facilities to manufacture them. Initial targets include high-entropy alloys, a promising class of metals that were discovered a few decades ago but have yet to be widely commercialized. These super-strong materials, made up of a half-dozen or so different elements, could be useful in turbine engines and even in fusion reactors.

Money: Raised $55 million in July 2025.

cuspai

periodic labs

LILA

RADICAL

https://www.technologyreview.com/2025/12/18/1130102/ai-materials-discovery/

…TO NOBEL PRIZES

K. Novoselov moved to NUS in 2019 to create **I-FIM – Institute for Functional Intelligent Materials.**

NUS National University of Singapore | Institute for Functional Intelligent Materials

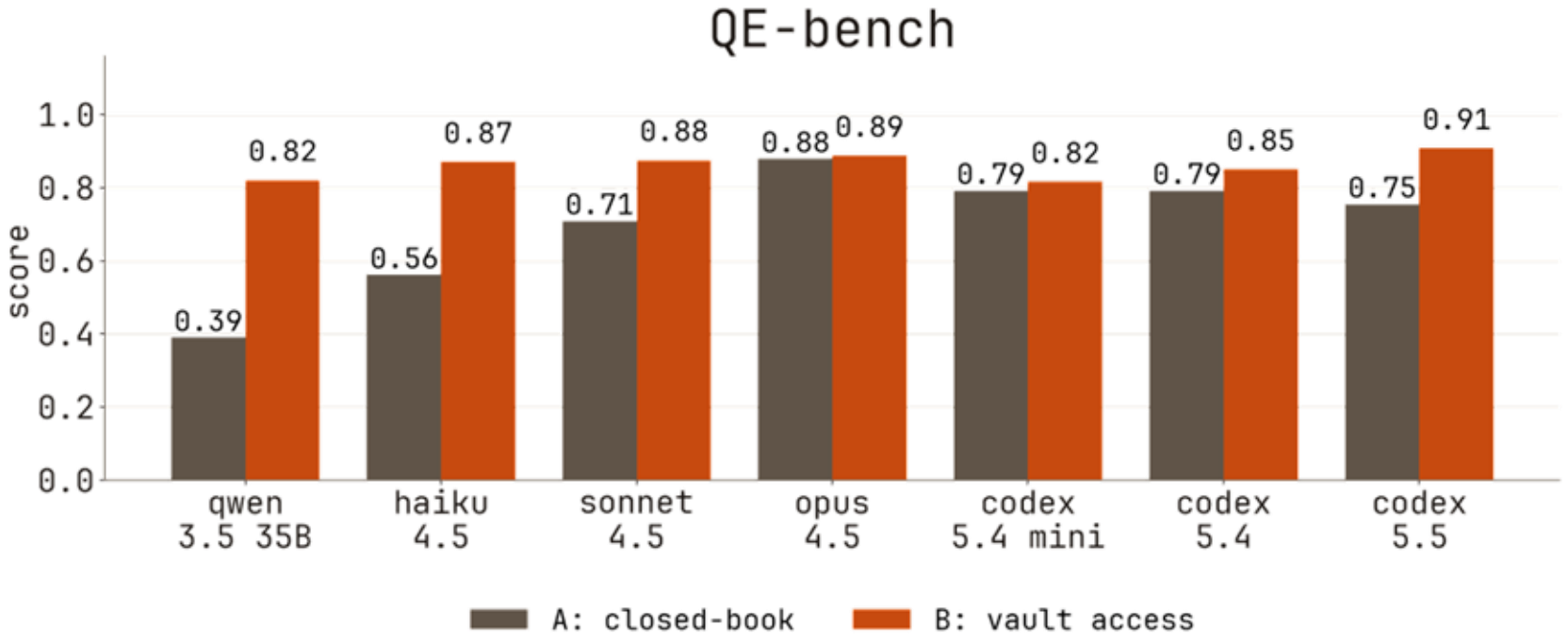
…**tight coupling between theory, algorithms and data …** the materials will be synthesised … using computational models, time-dependent machine learning and optimal control.

O. Yaghi moved to Tsinghua in 2026, to create a University-level AI Chemistry and Materials Research Institute, **AIMATRY (AI × Materials × Chemistry).**

… that will develop **forward-looking AI-enabled technologies for materials design and synthesis**, … **spanning the full chain from theory and computation to R&D and production**

THE BEST IS YET TO COME

- ML as the great accelerator
- LLM as knowledge integrators
- AI agents as drivers of simulations




THANK YOU ALL!
SwissTech Convention Center