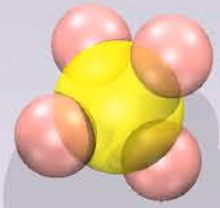
WORLD MATERIALS FORUM



MARVEL

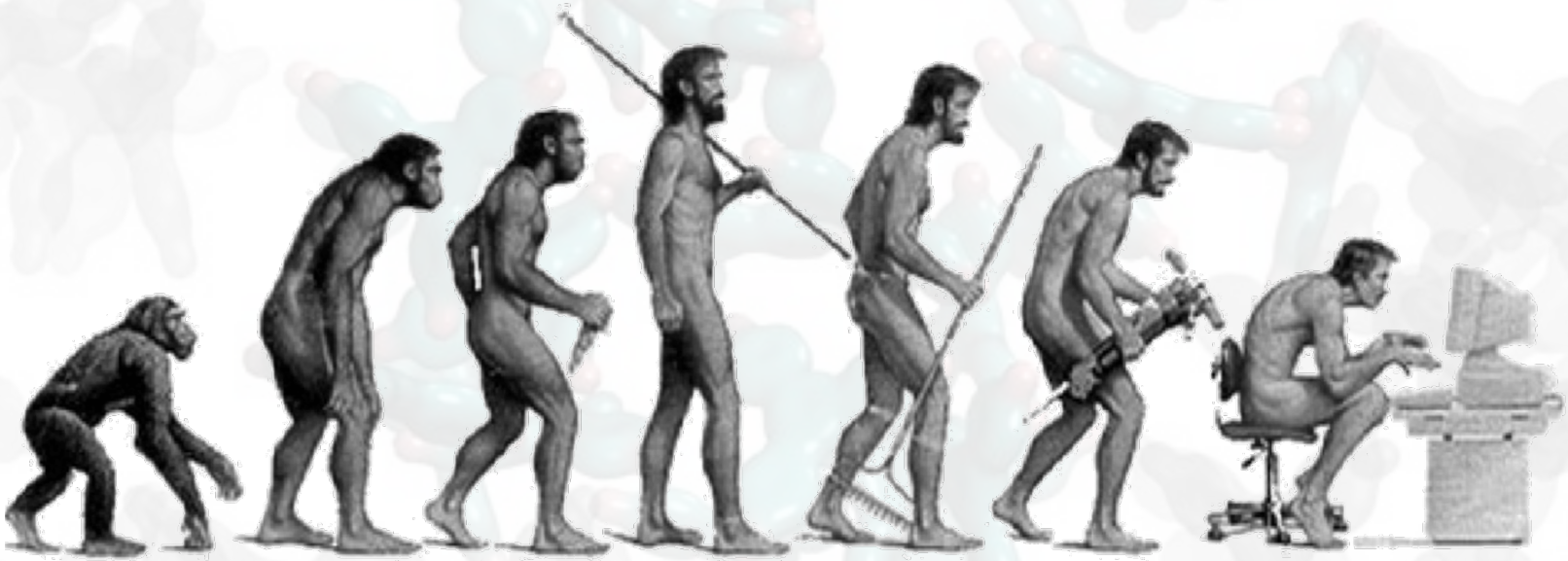
NATIONAL CENTRE OF COMPETENCE IN RESEARCH

AN INDUSTRIAL AGE FOR MATERIALS' SIMULATIONS

Nicola Marzari, EPFL

MATERIALS ARE KEY TO SOCIETAL WELL BEING

Human ages are named after materials - stone, bronze, iron, nuclear, silicon…

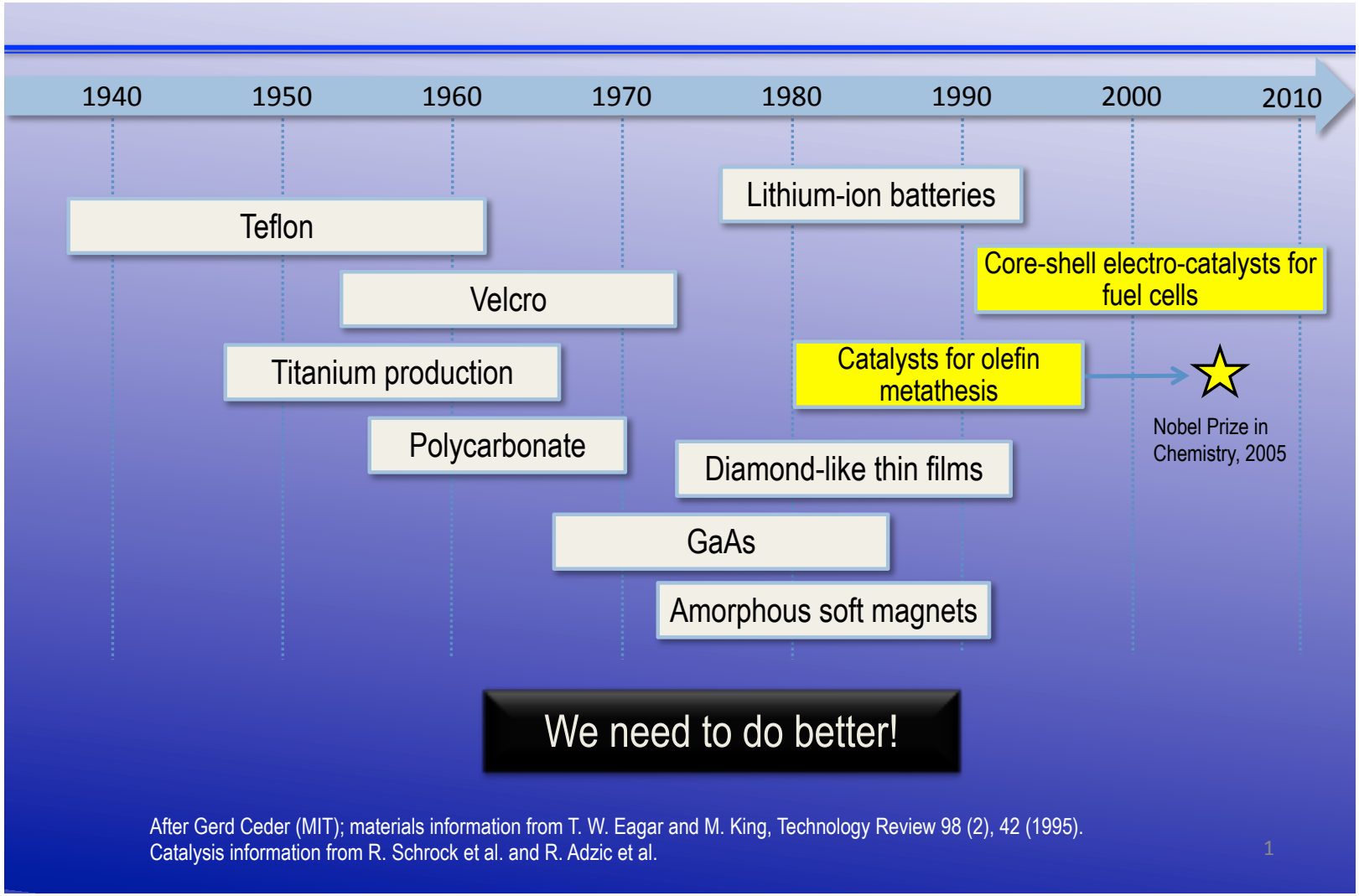


MATERIALS ARE KEY TO SOCIETAL WELL BEING

We need novel materials for:

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

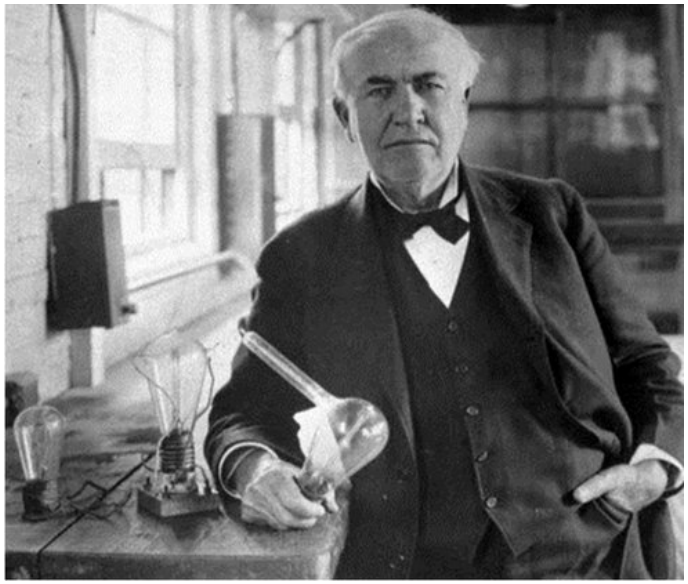
DISCOVERY TO APPLICATION IN THE 20th CENTURY



After Gerd Ceder (MIT); materials information from T. W. Eagar and M. King, Technology Review 98 (2), 42 (1995).
Catalysis information from R. Schrock et al. and R. Adzic et al.

MATERIALS' DEVELOPMENT: INTUITION, SEARCHES, AND SERENDIPITY

- Edison tested 3000 materials for his filament – settling on burned sewing thread.



MATERIALS' DEVELOPMENT: INTUITION, SEARCHES, AND SERENDIPITY

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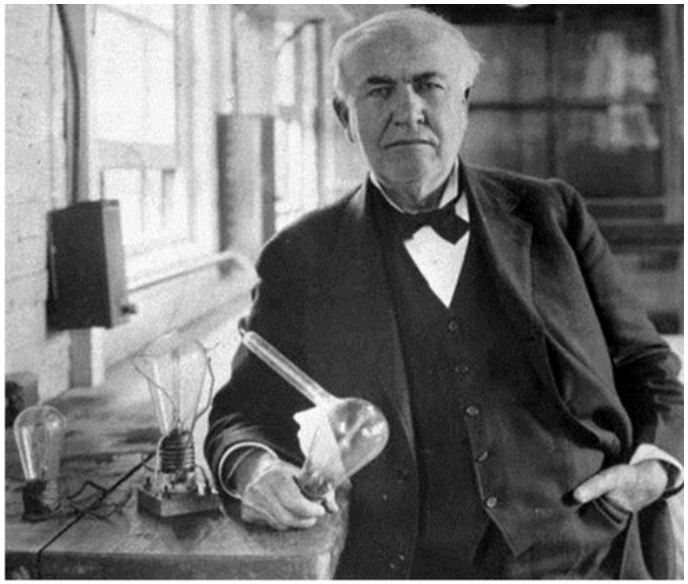

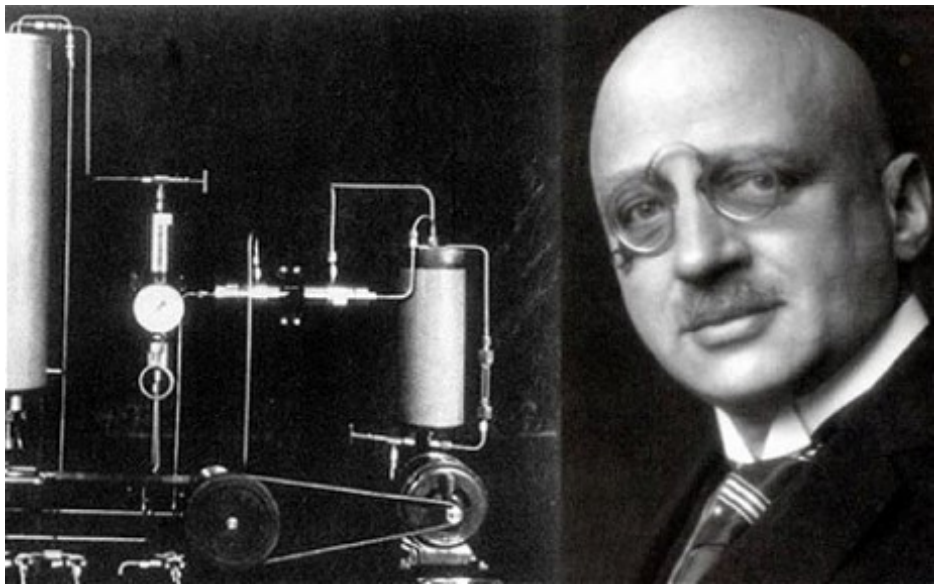

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- Norskov showed in 2009 that CoMo is a more efficient inexpensive catalyst.

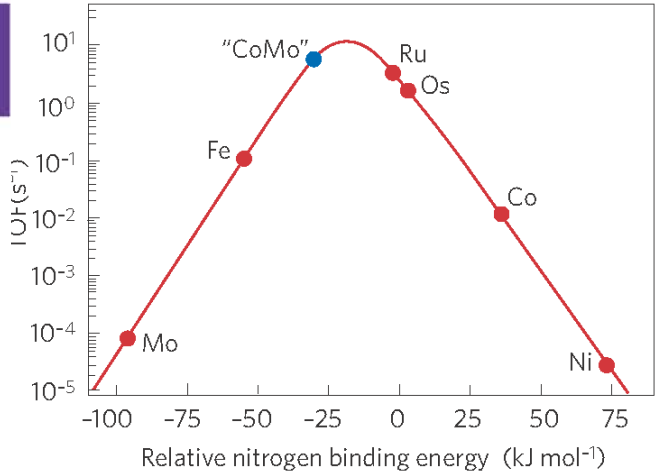
nature chemistry

REVIEW ARTICLE

PUBLISHED ONLINE: 19 MARCH 2009 | DOI: 10.1038/NCHEM.121

Towards the computational design of solid catalysts

J. K. Nørskov[1]*, T. Bligaard[1], J. Rossmeisl[1] and C. H. Christensen[2]



ACCELERATING TECHNOLOGY TRANSFER

- 2001: first-principles calculations show tunnelling magnetoresistance (TMR) in Fe/MgO/Fe junctions
- 2004: IBM and others show experimental TMR of 200%
- 2007: all hard drives shipped are based on TMR

THE RISE OF SIMULATION SCIENCE

2013 Chemistry Prize

Taking the Experiment to Cyberspace

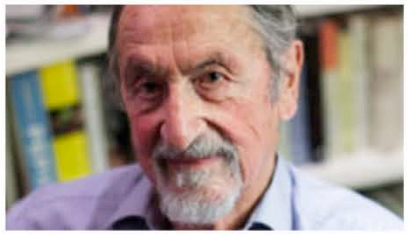


Photo © Harvard University

Martin Karplus

Martin Karplus, U.S. and Austrian citizen. Born 1930 in Vienna, Austria.

Photo: S. Fisch

Michael Levitt

Michael Levitt, U.S., British and Israeli citizen. Born 1947 in Pretoria,

Photo: Wikimedia Commons

Arieh Warshel

Arieh Warshel, U.S. and Israeli citizen. Born 1940 in Kibbutz Sde-

"The prize focuses on how to evaluate the variation in the energy of the real system in a accurate and efficient way […]. **The Car–Parrinello approach is the leading strategy along this line."**

"Simulations are so realistic that they predict the outcome of traditional experiments."

From www.nobelprize.org/nobel_prizes/chemistry/laureates/2013/

THE RISE OF SIMULATION SCIENCE

Inhomogeneous Electron Gas
P. Hohenberg and W. Kohn
Phys. Rev. **136**, B864 (9 November 1964)

Self-Consistent Equations Including Exchange and Correlation Effects
W. Kohn and L. J. Sham
Phys. Rev. **140**, A1133 (15 November 1965)

Nobel Focus: Chemistry by Computer

21 October 1998

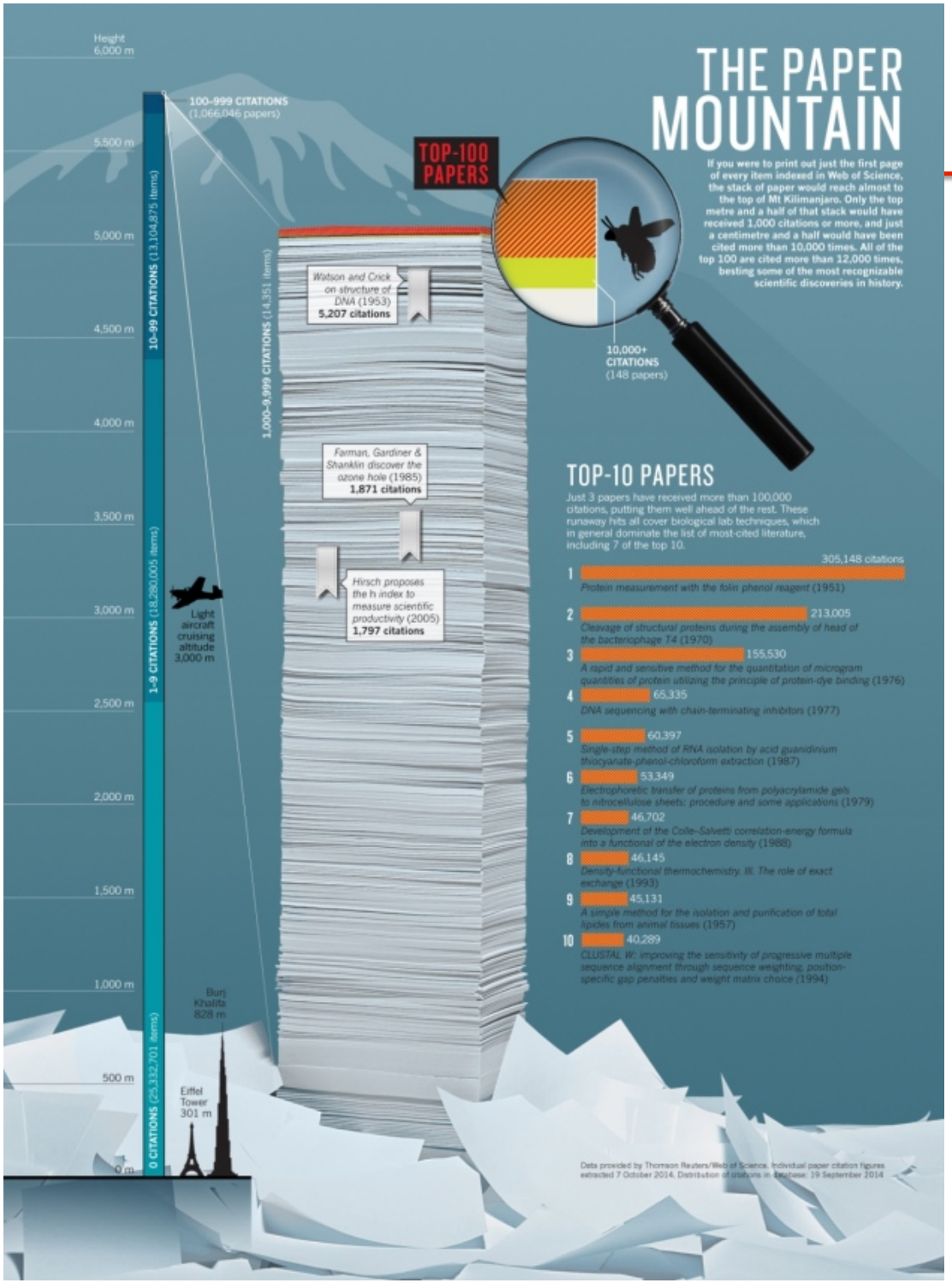
The 1998 Nobel Prize in chemistry recognizes two researchers whose work has allowed chemists to calculate the properties of molecules and solids on computers, without performing experiments in the lab. The basic principles of the calculation scheme were first described in *Physical Review* in the 1960s, and solid state physicists used them for decades before they became important in the chemistry world. The scheme drastically simplifies the solution of the quantum mechanical equations for a system of many electrons, and although approximate, the solutions are accurate enough that chemists can learn about large molecules without getting their hands wet.

Calculations made easy. Localized orbitals in the electronic structure of the $BaTiO_3$ crystal, calculated using density functional theory, which was invented by 1998 Nobel Laureate Walter Kohn.

Nicola Marzari and David Vanderbilt/Rutgers University

MOST CITED PAPERS IN APS (FROM 1893)

	Journal	# cites	Title	Author(s)
1	PRB (1988)	39190	Development of the Colle-Salvetti Correlation-Energy …	Lee, Yang, Parr
2	PRL (1996)	25452	Generalized Gradient Approximation Made Simple	Perdew, Burke, Ernzerhof
3	PRA (1988)	22904	Density-Functional Exchange-Energy Approximation …	Becke
4	PR (1965)	20142	Self-Consistent Equations Including Exchange and Correlation …	Kohn and Sham
5	PRB (1996)	13731	Efficient Iterative Schemes for Ab Initio Total-Energy …	Kresse and Furthmuller
6	PRB (1976)	13160	Special Points for Brillouin-Zone Integrations	Monkhorst and Pack
7	PRB (1992)	10876	Accurate and Simple Analytic Representation of the Electron …	Perdew and Wang
8	PRB (1999)	10007	From Ultrasoft Pseudopotentials to the Projector Augmented …	Kresse and Joubert
9	PRB (1990)	9840	Soft Self-Consistent Pseudopotentials in a Generalized …	Vanderbilt
10	PR (1964)	9789	Inhomogeneous Electron Gas	Hohenberg and Kohn
11	PRB (1981)	9787	Self-Interaction Correction to Density-Functional Approx. …	Perdew and Zunger
12	PRB (1992)	9786	Atoms, Molecules, Solids, and Surfaces - Applications of the …	Perdew, Chevary, …
13	PRB (1986)	9313	Density-Functional Approx. for the Correlation-Energy …	Perdew
14	PR (1934)	9271	Note on an Approximation Treatment for Many-Electron Systems	Moller and Plesset
15	PRB (1994)	9100	Projector Augmented-Wave Method	Blochl
16	PRL (1980)	7751	Ground-State of the Electron-Gas by a Stochastic Method	Ceperley and Alder
17	PRL (1987)	7663	Inhibited Spontaneous Emission in Solid-State Physics …	Yablonovitch
18	PRL (1986)	7589	Atomic Force Microscope	Binnig, Quate, Gerber
19	PRB (1991)	7425	Efficient Pseudopotentials for Plane-Wave Calculations	Troullier and Martins
20	PRB (1993)	6925	Ab initio Molecular Dynamics for Liquid Metals	Kresse and Hafner
21	PR (1961)	6467	Effects of Configuration Interaction on Intensities and Phase Shifts	Fano
22	PR (1957)	6260	Theory of Superconductivity	Bardeen, Cooper, Schrieffer

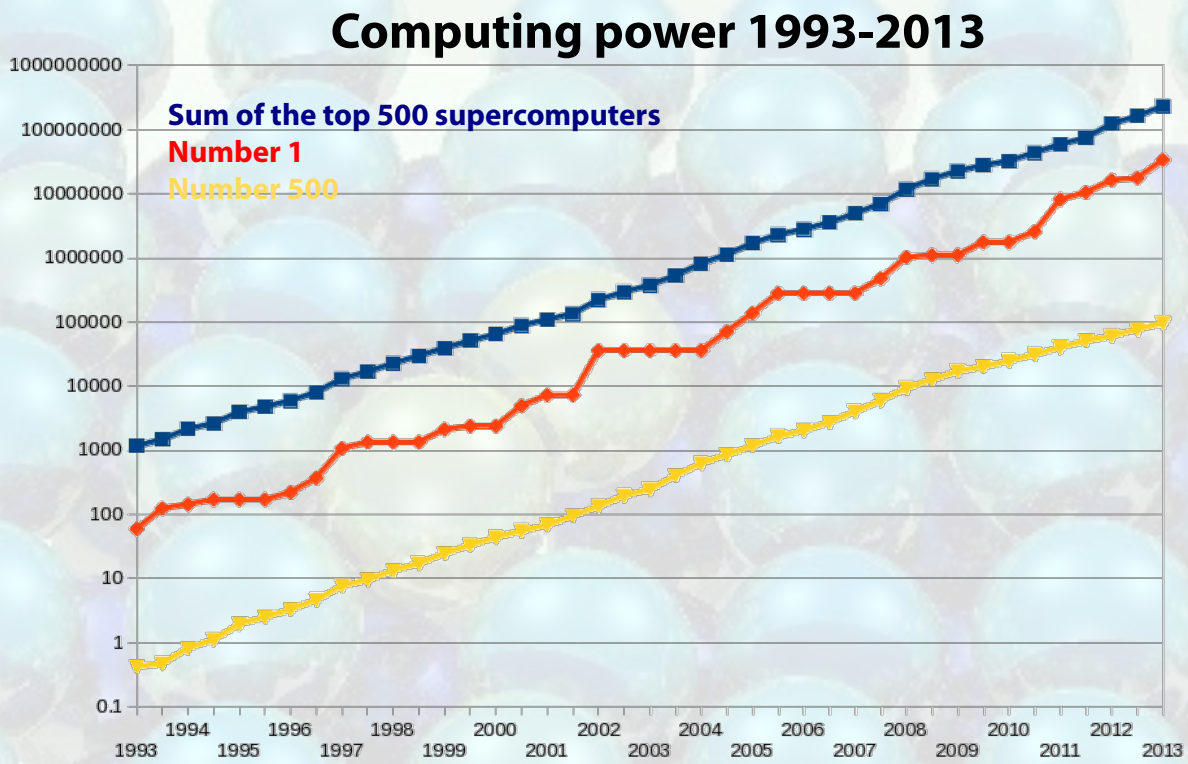


NATURE,
October 2014

THE TOP 100 PAPERS:

12 papers on quantum simulations in the top-100 most cited papers in the entire scientific literature, ever.

THROUGHPUT CAPACITY DOUBLES EVERY 14 MONTHS



If brick-and-mortar laboratories were to follow this pace, an experiment that took **one year in 1986** would take **one second in 2015** (30-million-fold increase)

REVOLUTION, NOT EVOLUTION

So, what would happen if the accuracy and speed of our experiments were to increase at the speed of information-and-communication technologies?

A revolution in scientific discovery and technological development

WORLDWIDE DRIVE: THE MATERIALS GENOME INITIATIVE

nature materials
REVIEW ARTICLE
PUBLISHED ONLINE: 20 FEBRUARY 2013 | DOI: 10.1038/NMAT3568

The high-throughput highway to computational materials design

LETTERS

Where are nature's missing structures?

GUS L. W. HART
Department of Physics & Astronomy, Brigham Young University, Provo, Utah 84602, USA
e-mail: gus.hart@gmail.com

editorial

Fuelling discovery by sharing

The United States Materials Genome Initiative aims at accelerating the discovery, development and deployment of materials. Yet, finding data standards and sharing practices that can be leveraged by the disparate communities in materials science and technology may prove difficult.

GRC Gordon Research Conferences
Frontiers of Science

Conference Program

HOME
CONFERENCES
- Current Meetings (2013)
- Upcoming Meetings (2014)

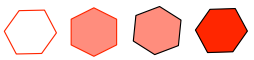
High Pressure, Research at

June 24-29, 2012
University of New England
Biddeford, ME

MEETING LINKS
- Conference History
- Contact Chairs

SUNDAY

2:00 pm - 9:00 pm	Arrival and Check-in (Office Closed 6:00 pm - 7:00 pm)
6:00 pm	Dinner
7:30 pm - 7:40 pm	Welcome / Introductory Comments by GRC Site Staff
7:40 pm - 9:30 pm	**Structural Predictions at Extreme Conditions: Are Experiments Still Necessary?** Discussion Leader: **John Tse** (University of Saskatoon)



CONCLUSIONS

We plan to **transform and accelerate invention and discovery in science and technology**, and especially to transform and accelerate the design and discovery of novel materials.

We will achieve this objective by exploiting:

- the predictive accuracy of quantum simulations
- Moore's law for resources (doubling every 14 months)
- the powerful synergy of modeling and simulation with the ideas and tools of computer science