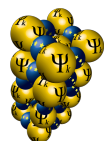




Introduction to AiiDA

Writing reproducible workflows using AiiDA
May 21st-24th, 2019, Lausanne



swissuniversities



THE RISE OF SIMULATION SCIENCE

2013 Chemistry Prize



**Taking the
Experiment to
Cyberspace**

The Nobel Prize in Chemistry 2013



Photo © Harvard University

Martin Karplus

Martin Karplus, U.S. and Austrian citizen. Born 1930 in Vienna, Austria. Ph.D. 1952 from California Institute



Photo: S. Fisch

Michael Levitt

Michael Levitt, U.S., British and Israeli citizen. Born 1947 in Pretoria, South Africa. Ph.D. 1971 from



Photo: Wikimedia Commons

Arie Warshel

Arie Warshel, U.S. and Israeli citizen. Born 1940 in Kibbutz Sde-Nahum, Israel. Ph.D. 1969 from

“The prize focuses on how to evaluate the variation in the energy of the real system in a accurate and efficient way.”

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

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



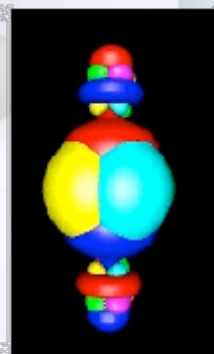
Inhomogeneous Electron Gas
P. Hohenberg and W. Kohn
Phys. Rev. **136**, B864 (9 November 1964)

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.

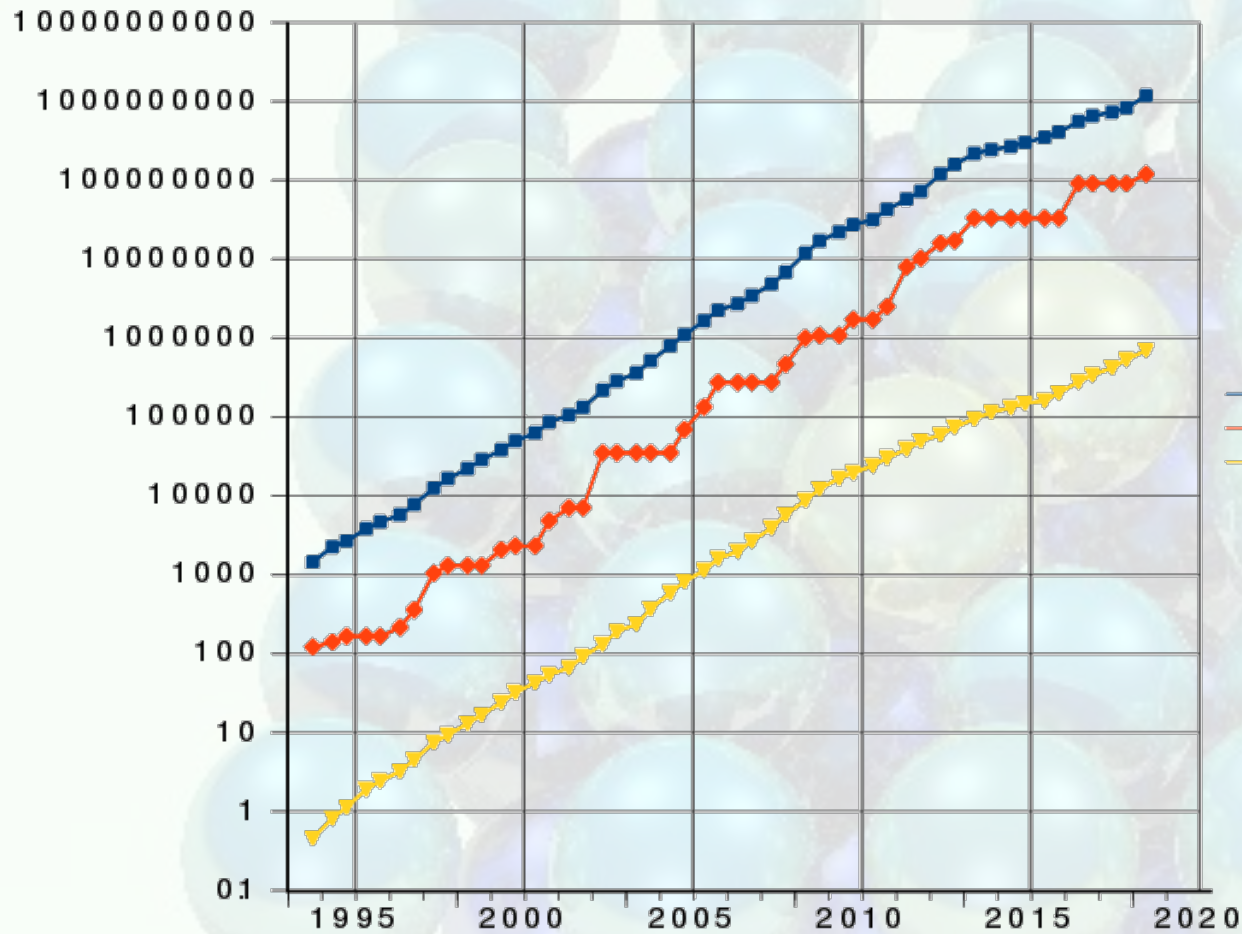


Calculations made easy. Localized orbitals in the electronic structure of the BaTiO_3 crystal, calculated using density functional theory, which was invented by 1998 Nobel Laureate Walter Kohn.

Nicola Marzari and David Vanderbilt/Rutgers University



THE ENGINE



Computing power 1993-2018

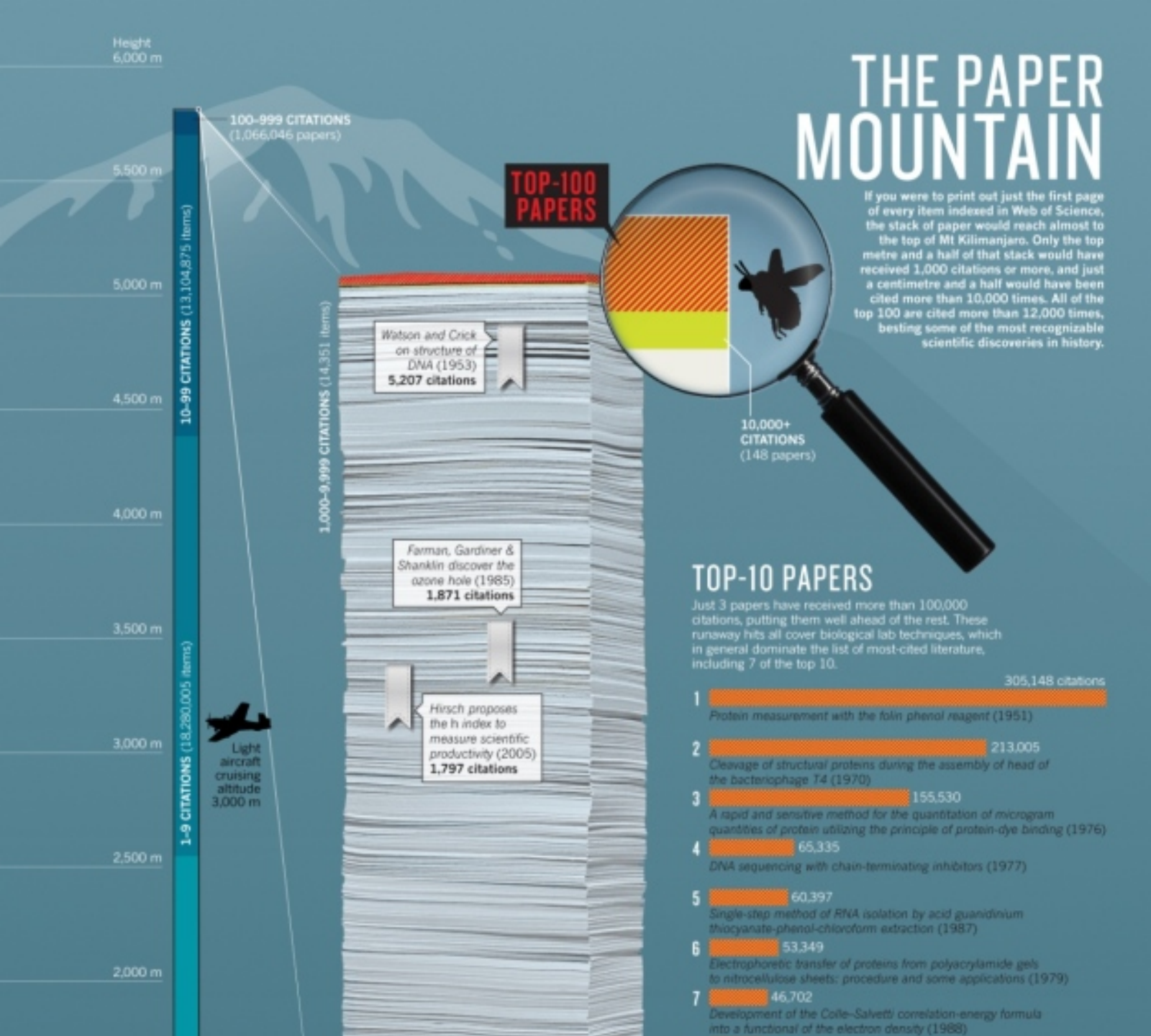
Sum of the top 500 supercomputers
Number 1
Number 500

Sum
Top
#500

If brick-and-mortar laboratories were to follow this pace, an experiment that took **one year in 1989** would take **one second in 2018** (30-million-fold increase)



THE TOP 100 PAPERS: 12 papers on density- functional theory in the top-100 most cited papers in the entire scientific literature, ever.



MOST CITED PAPERS IN THE HISTORY OF APS

	Journal	# cites	Title	Author(s)
1	PRL (1996)	78085	Generalized Gradient Approximation Made Simple	Perdew, Burke, Ernzerhof
2	PRB (1988)	67303	Development of the Colle-Salvetti Correlation-Energy ...	Lee, Yang, Parr
3	PRB (1996)	41683	Efficient Iterative Schemes for Ab Initio Total-Energy ...	Kresse and Furthmuller
4	PR (1965)	36841	Self-Consistent Equations Including Exchange and Correlation ...	Kohn and Sham
5	PRA (1988)	36659	Density-Functional Exchange-Energy Approximation ...	Becke
6	PRB (1976)	31865	Special Points for Brillouin-Zone Integrations	Monkhorst and Pack
7	PRB (1999)	30940	From Ultrasoft Pseudopotentials to the Projector Augmented ...	Kresse and Joubert
8	PRB (1994)	30801	Projector Augmented-Wave Method	Bloch
9	PR (1964)	30563	Inhomogeneous Electron Gas	Hohenberg and Kohn
10	PRB (1993)	19903	Ab initio Molecular Dynamics for Liquid Metals	Kresse and Hafner
11	PRB (1992)	17286	Accurate and Simple Analytic Representation of the Electron ...	Perdew and Wang
12	PRB (1990)	15618	Soft Self-Consistent Pseudopotentials in a Generalized ...	Vanderbilt
13	PRB (1992)	15142	Atoms, Molecules, Solids, and Surfaces - Applications of the ...	Perdew, Chevary, ...
14	PRB (1981)	14673	Self-Interaction Correction to Density-Functional Approx. ...	Perdew and Zunger
15	PRB (1986)	13907	Density-Functional Approx. for the Correlation-Energy ...	Perdew
16	RMP (2009)	13513	The Electronic Properties of Graphene	Castro Neto et al.
17	PR (1934)	12353	Note on an Approximation Treatment for Many-Electron Systems	Moller and Plesset
18	PRB (1972)	11840	Optical Constants on Noble Metals	Johnson and Christy
19	PRB (1991)	11580	Efficient Pseudopotentials for Plane-Wave Calculations	Troullier and Martins
20	PRL (1980)	10784	Ground-State of the Electron-Gas by a Stochastic Method	Ceperley and Alder



THREE THINGS TO REMEMBER



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- 1) Science in the 21st century will be dominated by computational science and data/machine learning



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- 2) It's a great model, where knowledge and tools can be disseminated worldwide at no cost (so, it's also a globalized and liquid science)



THREE THINGS TO REMEMBER

- 1) Science in the 21st century will be dominated by computational science and data/machine learning
- 2) It's a great model, where knowledge and tools can be disseminated worldwide at no cost (so, it's also a globalized and liquid science)
- 3) We do not have a development model for computational science



OPEN SCIENCE PLATFORM

- Our definition of an Open Science Platform [1]:
 - **Open simulation codes**
 - **Open architecture** to manage simulations and **open workflows**
 - Support for **Open Data, Data Management Plans** and FAIR-compliant sharing
 - **Straightforward availability** of the tools, with **curated open-data services** enabling turn-key workflows (pseudopotential libraries, ...)

[1] Pizzi G. (2018) *Open-Science Platform for Computational Materials Science: AiiDA and the Materials Cloud*. In: Andreoni W., Yip S. (eds), *Handbook of Materials Modeling* (Springer, Cham).



OUR GOAL

Build an open-science infrastructure
with computational services offered
to scientific, industrial community and beyond

Like a synchrotron, but for
open and reproducible simulations

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In: Andreoni W., Yip S. (eds), *Handbook of Materials Modeling* (Springer, Cham).



CORE INFRASTRUCTURE

Open-source software



<http://aiida.net>



<http://materialscloud.org>



CORE INFRASTRUCTURE

AiiDA as the “operating system” to manage,
automate and store simulations and their results

and

Materials Cloud as the open-science
dissemination portal and cloud simulation platform

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