




**Digital chemistry:  
Paradigm shift,  
cultural evolution  
or business as usual?**

**Jeremy Frey**

University of Southampton  
Head Computational Systems Chemistry



# Digital chemistry: Paradigm shift, cultural evolution or business as usual?

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25/09/2024

ChemTalk Basel 2024



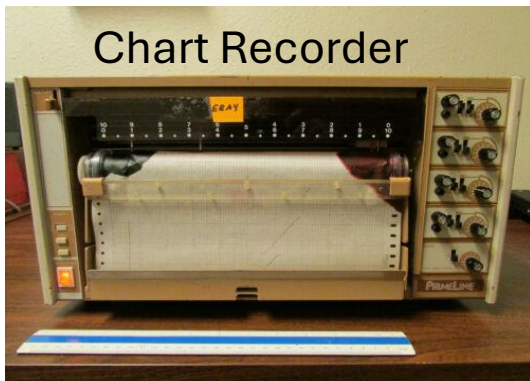
# Vision



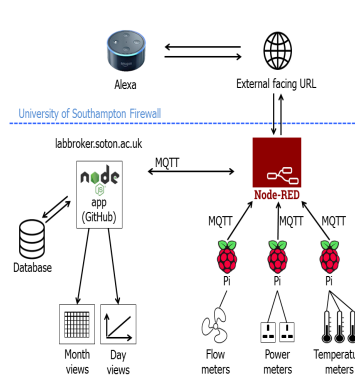
Science  
What we investigate

Digital Technoscape  
How we investigate

Yes! We did do experiments before computers!



<http://news.bbc.co.uk/1/hi/sci/tech/4233757.stm>



The progress of digitalization of my research

Pre-Digital Computers

Physical model of the Solent basin



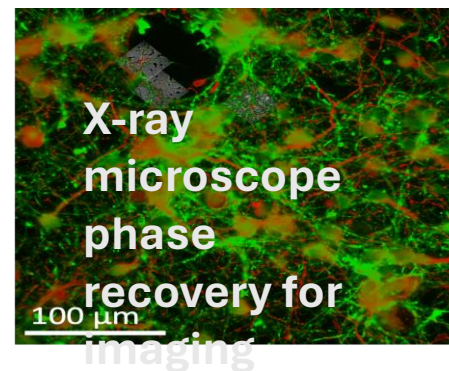
By Francois-Xavier Beckers, CC BY 3.0, <https://commons.wikimedia.org/w/index.php?curid=32926674>

Computers are useful



[https://en.wikipedia.org/wiki/BBC\\_Micro](https://en.wikipedia.org/wiki/BBC_Micro)

Computers are essential



X-ray microscope phase recovery for imaging

Computers take over – AI Scientist?



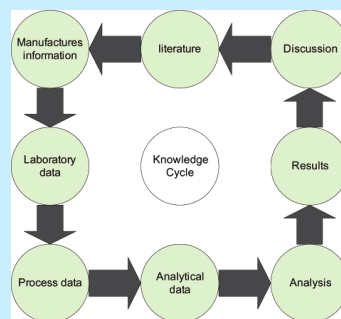
Robotic Labs?

2004

## Dark Lab or Smart Lab: The Challenges for 21st Century Laboratory Software

Abstract:

Introduction



## Dark Lab or Smart Lab: The challenges for 21<sup>st</sup> Century Laboratory Software, Frey 2004

The Paperless Office or Paperless Laboratory Syndrome

2024

Digital  
Discovery



PERSPECTIVE

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Cite this: DOI: 10.1039/d4dd00130c

## Digital chemistry: navigating the confluence of computation and experimentation – definition, status quo, and future perspective

Stefan Bräse <sup>1a,b</sup>

Digital chemistry represents a transformative approach integrating computational methods, digital data, and automation within the chemical sciences. It is defined by using digital toolkits and algorithms to simulate, predict, accelerate, and analyze chemical processes and properties, augmenting traditional experimental methods. The current status quo of digital chemistry is marked by rapid advancements in several key areas: high-throughput screening, machine learning models, quantum chemistry, and laboratory automation. These technologies have enabled unprecedented speeds in discovering and optimizing new molecules, materials, and reactions. Digital retrosynthesis and structure–active prediction tools have supported these endeavors. Furthermore, integrating large-language models and robotics in chemistry labs (e.g. demonstrated in self-driving labs) have begun to automate routine tasks and complex decision-making processes. Looking forward, the future of digital and digitalized chemistry is poised for significant growth, driven by the increasing accessibility of computational resources, the expansion of chemical databases, and the refinement of artificial intelligence algorithms. This evolution promises to accelerate innovation in drug discovery, materials science, and sustainable manufacturing, ultimately leading to more efficient, cost-effective, and environmentally friendly chemical research and production. The challenge lies in advancing the technology itself, fostering interdisciplinary collaboration, and ensuring the ethical use of digital tools in chemical research.

Received 13th May 2024  
Accepted 15th August 2024  
DOI: 10.1039/d4dd00130c  
rsc.li/digitaldiscovery



## Digital chemistry: navigating the confluence of computation and experimentation – definition, status quo, and future perspectives, Bräse 2024

time.

(II) Growth of computational power (the 1970s–1980s):

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<sup>b</sup>Institute for Biological and Chemical Systems – IBCS-FMS, Karlsruhe Institute of Technology, Kaiserstrasse 12, 76131 Karlsruhe, Germany

compounds with their biological activities. This was a major step forward in drug design, allowing for the prediction of the activity of new compounds before their synthesis.

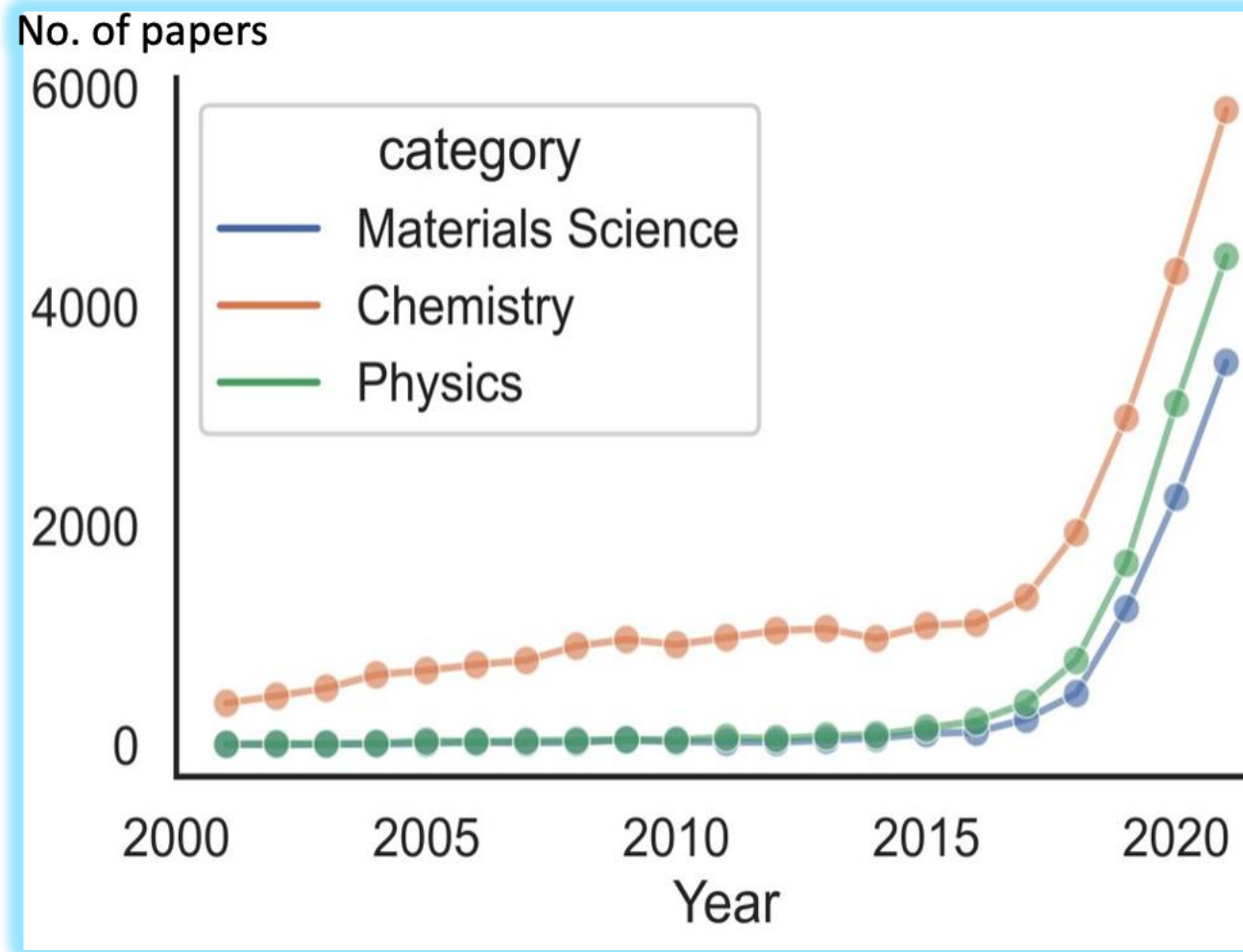
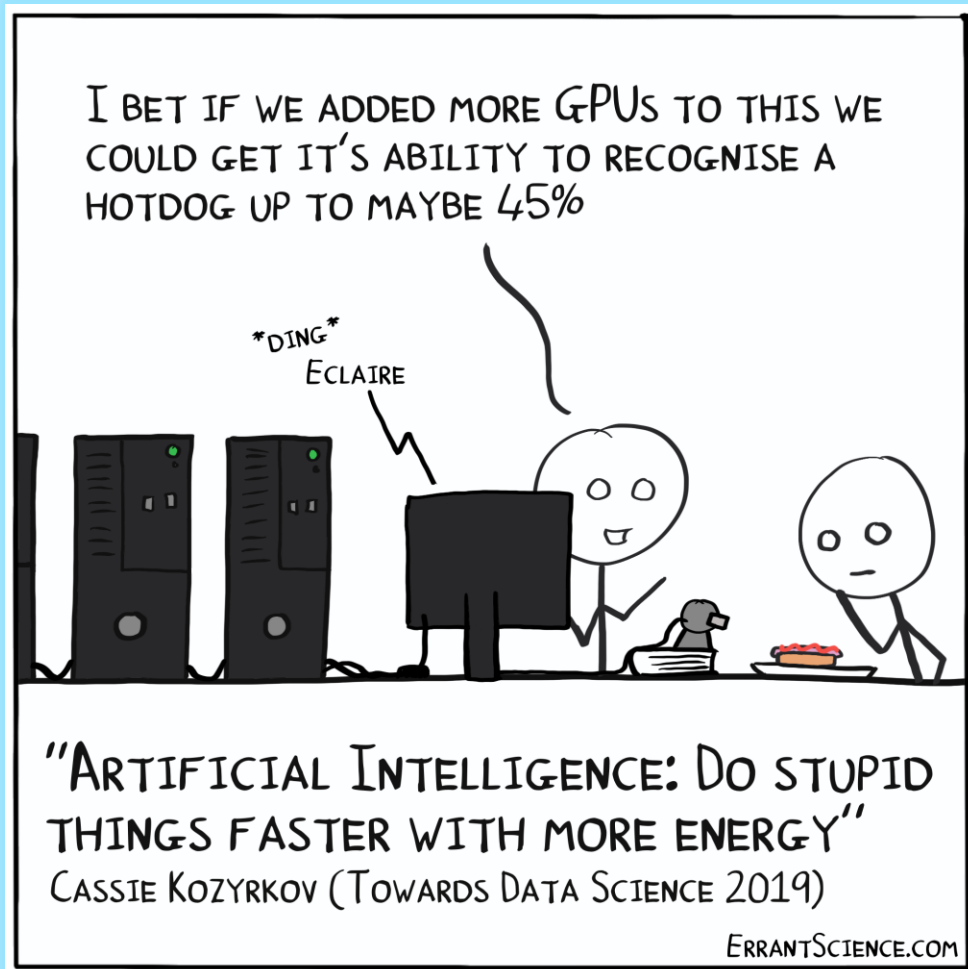
(IV) Rise of high-throughput screening and robotics (1990s–2000s):

The integration of high-throughput experimentation (HTE) and screening (HTS) technologies and robotics in the 1990s and

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Digital Discovery

# Augmented Chemical Intelligence?

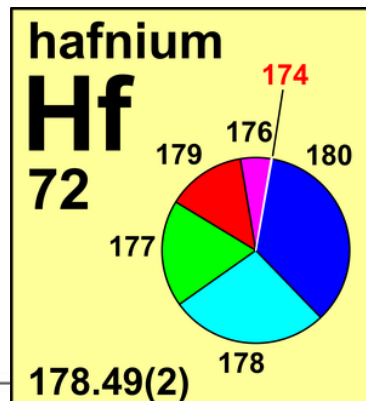
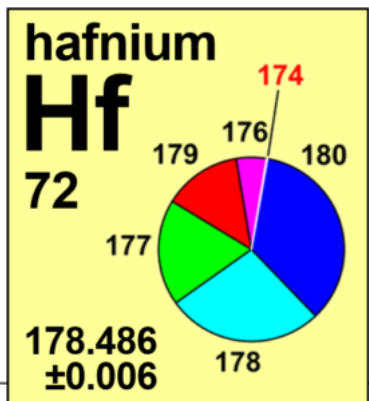


# Data Driven Science

## IUPAC Periodic Table of the Elements

1 <b>H</b> hydrogen 1.0080 ± 0.0002																	18 <b>He</b> helium 4.0026 ± 0.0001	
3 <b>Li</b> lithium 6.94 ± 0.06	4 <b>Be</b> beryllium 9.0122 ± 0.0001																	10 <b>Ne</b> neon 20.180 ± 0.001
11 <b>Na</b> sodium 22.990 ± 0.001	12 <b>Mg</b> magnesium 24.305 ± 0.002																	18 <b>Ar</b> argon 39.95 ± 0.16
19 <b>K</b> potassium 39.098 ± 0.001	20 <b>Ca</b> calcium 40.078 ± 0.004	21 <b>Sc</b> scandium 44.956 ± 0.001	22 <b>Ti</b> titanium 47.867 ± 0.001	23 <b>V</b> vanadium 50.942 ± 0.001	24 <b>Cr</b> chromium 51.996 ± 0.001	25 <b>Mn</b> manganese 54.938 ± 0.001	26 <b>Fe</b> iron 55.845 ± 0.002	27 <b>Co</b> cobalt 58.933 ± 0.001	28 <b>Ni</b> nickel 58.693 ± 0.001	29 <b>Cu</b> copper 63.546 ± 0.003	30 <b>Zn</b> zinc 65.38 ± 0.02	31 <b>Ga</b> gallium 69.723 ± 0.001	32 <b>Ge</b> germanium 72.630 ± 0.008	33 <b>As</b> arsenic 74.922 ± 0.001	34 <b>Se</b> selenium 78.971 ± 0.008	35 <b>Br</b> bromine 79.904 ± 0.003	36 <b>Kr</b> krypton 83.798 ± 0.002	
37 <b>Rb</b>	38 <b>Sr</b>	39 <b>Y</b>	40 <b>Zr</b>	41 <b>Nb</b> niobium 92.906 ± 0.001	42 <b>Mo</b> molybdenum 95.95 ± 0.01	43 <b>Tc</b> technetium [97]	44 <b>Ru</b> ruthenium 101.07 ± 0.02	45 <b>Rh</b> rhodium 102.91 ± 0.01	46 <b>Pd</b> palladium 106.42 ± 0.01	47 <b>Ag</b> silver 107.87 ± 0.01	48 <b>Cd</b> cadmium 112.41 ± 0.01	49 <b>In</b> indium 114.82 ± 0.01	50 <b>Sn</b> tin 118.71 ± 0.01	51 <b>Sb</b> antimony 121.76 ± 0.01	52 <b>Te</b> tellurium 127.60 ± 0.03	53 <b>I</b> iodine 126.90 ± 0.01	54 <b>Xe</b> xenon 131.29 ± 0.01	
				73 <b>Ta</b> tantalum 180.95 ± 0.01	74 <b>W</b> tungsten 183.84 ± 0.01	75 <b>Re</b> rhenium 186.21 ± 0.01	76 <b>Os</b> osmium 190.23 ± 0.03	77 <b>Ir</b> iridium 192.22 ± 0.01	78 <b>Pt</b> platinum 195.08 ± 0.02	79 <b>Au</b> gold 196.97 ± 0.01	80 <b>Hg</b> mercury 200.59 ± 0.01	81 <b>Tl</b> thallium 204.38 ± 0.01	82 <b>Pb</b> lead 207.2 ± 1.1	83 <b>Bi</b> bismuth 208.98 ± 0.01	84 <b>Po</b> polonium [209]	85 <b>At</b> astatine [210]	86 <b>Rn</b> radon [222]	
				105 <b>Db</b> dubnium [268]	106 <b>Sg</b> seaborgium [269]	107 <b>Bh</b> bohrium [270]	108 <b>Hs</b> hassium [269]	109 <b>Mt</b> meitnerium [277]	110 <b>Ds</b> darmstadtium [281]	111 <b>Rg</b> roentgenium [282]	112 <b>Cn</b> copernicium [285]	113 <b>Nh</b> nihonium [286]	114 <b>Fl</b> flerovium [290]	115 <b>Mc</b> moscovium [290]	116 <b>Lv</b> livermorium [293]	117 <b>Ts</b> tennessine [294]	118 <b>Og</b> oganeson [294]	
				58 <b>Ce</b> cerium 140.12 ± 0.01	59 <b>Pr</b> praseodymium 140.91 ± 0.01	60 <b>Nd</b> neodymium 144.24 ± 0.01	61 <b>Pm</b> promethium [145]	62 <b>Sm</b> samarium 150.36 ± 0.02	63 <b>Eu</b> europium 151.96 ± 0.01	64 <b>Gd</b> gadolinium 157.25 ± 0.03	65 <b>Tb</b> terbium 158.93 ± 0.01	66 <b>Dy</b> dysprosium 162.50 ± 0.01	67 <b>Ho</b> holmium 164.93 ± 0.01	68 <b>Er</b> erbium 167.26 ± 0.01	69 <b>Tm</b> thulium 168.93 ± 0.01	70 <b>Yb</b> ytterbium 173.05 ± 0.02	71 <b>Lu</b> lutetium 174.97 ± 0.01	
				90 <b>Th</b> thorium 232.04 ± 0.01	91 <b>Pa</b> protactinium 231.04 ± 0.01	92 <b>U</b> uranium 238.03 ± 0.01	93 <b>Np</b> neptunium [237]	94 <b>Pu</b> plutonium [244]	95 <b>Am</b> americium [243]	96 <b>Cm</b> curium [247]	97 <b>Bk</b> berkelium [247]	98 <b>Cf</b> californium [251]	99 <b>Es</b> einsteinium [252]	100 <b>Fm</b> fermium [257]	101 <b>Md</b> mendelevium [258]	102 <b>No</b> nobelium [259]	103 <b>Lr</b> lawrencium [262]	

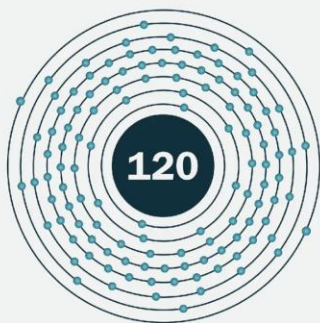
Key:  
atomic number  
**Symbol**  
name  
abbreviated standard  
atomic weight



NEWS CHEMISTRY

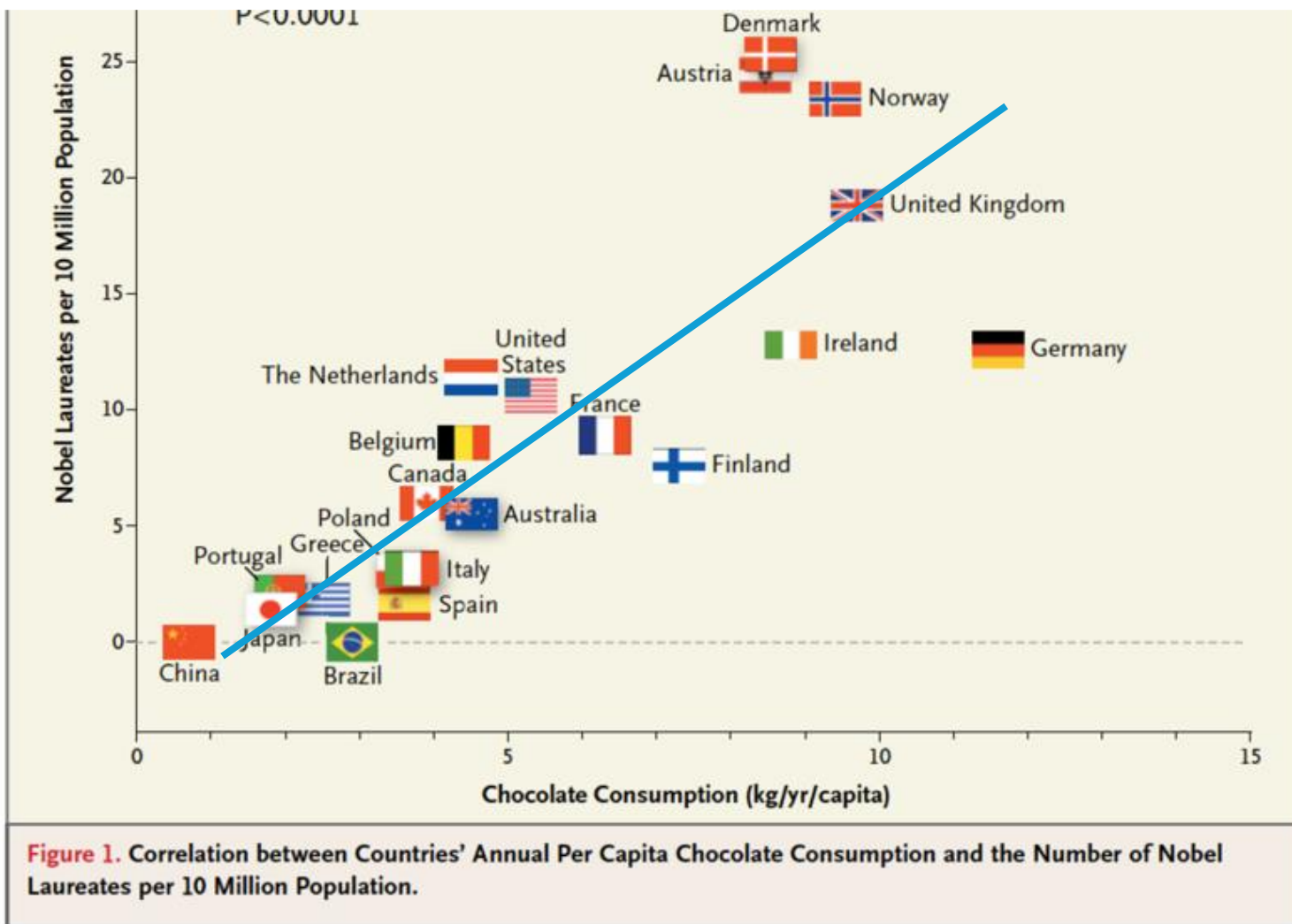
### A new element on the periodic table might be within reach

Scientists made a known element with a new technique, opening up possibilities



# Correlations

# Chocolate and Nobel Prizes



## THE SIX POLYMORPHS OF CHOCOLATE

The molecules in cocoa butter can be stacked together in different ways - these are known as 'polymorphs'. Tempering chocolate is required to obtain only form V, the most desirable. This is achieved by allowing the chocolate to cool at room temperature, which leads to some of all the polymorphs except VI forming, then heating gently to just below the melting point of form V, so it is the major form remaining.

FORM & MELTING POINT	DESCRIPTION & PROPERTIES
<b>I</b> 17.3 °C	<b>BOTH SOFT AND CRUMBLY WITH NOTICEABLE BLOOMING</b> Form I is produced by cooling melted chocolate rapidly (e.g. by putting it in the freezer).
<b>II</b> 23.3 °C	Form II is produced by cooling melted chocolate at 2°C per minute. Form I crystals also gradually become Form II after a short time of freezing temperature storage.
<b>III</b> 25.5 °C	<b>BOTH FIRM, BUT DON'T GIVE A GOOD 'SNAP', AND SHOW SOME BLOOMING</b> Form III is produced by cooling at 5-10°C. Form II becomes Form III after storage at low temperatures above freezing.
<b>IV</b> 27.3 °C	Form IV is produced by allowing melted chocolate to cool at room temperature; Form III also becomes Form IV after storage at room temperature for some time.
<b>V</b> 33.8 °C	<b>SHINY, SMOOTH TEXTURE, GOOD 'SNAP', AND MELTS IN THE MOUTH</b> Formed by tempering chocolate slowly at room temperature. Most desirable!
<b>VI</b> 36.3 °C	<b>HARD AND MELTS SLOWLY IN THE MOUTH, SHOWS SOME BLOOMING</b> Can't be formed from melted chocolate - can only be formed after solid, tempered chocolate has rested for at least 4 months.

**INCREASED STABILITY & DENSITY**

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# Water surface is acidic

Victoria Buch\*,

\*Fritz Haber Institute  
5250, Centre National  
Biochemistry, Academi  
Czech Republic; and

Edited by Mark A. R.

Water autoionization is a process of basic ions. However, pH of water is lower, the reduction of the surface. The evidence from molecular dynamics and OH<sup>-</sup> ions, derived from spectroscopic isotopies at the surface. H<sub>3</sub>O<sup>+</sup> does, but OH<sup>-</sup> the H<sub>2</sub>O surface is reasons, the strength is expected to increase. have a significant atmosphere.

density functional theory water autoionization

In room-temperature autoionized, yielding ionization in crystal ice to water, ice is a (1). As recently revealed, aqueous surface: therefore, autoionization

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### Featured Research

from universities, journals, and other organizations

## Rewrite the textbooks on water's surface tension: Air-water interface is negatively charged by the adsorption of hydroxide ions

Date: March 19, 2014

Source: University of Melbourne

Summary: Researchers in Australia make significant difference in water used by the next biophysicists and engineers. latest investigations have the physical Chemistry charged by the adsorption

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### Related Topics

#### Matter & Energy

- > Nature of Water
- > Chemistry
- > Inorganic Chemistry
- > Thermodynamics
- > Biochemistry
- > Nuclear Energy

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These long-term Chem negat

Prof A Depar "The : chang



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Chemistry and  
610 6 Prague,

006)

constant volume and dynamics simulations of H<sub>3</sub>O<sup>+</sup> and OH<sup>-</sup> on was carried out for a slab with two open is "on-the-fly" technon transfer systems d transitions between automatically included e high computational l system, the duration

PAPER

[www.rsc.org/faraday\\_d](http://www.rsc.org/faraday_d) | Faraday Discussions

## The surface of neat water is basic

James K. Beattie,\* Alex M. Djerdjev and Gregory G. Warr

Received 28th March 2008, Accepted 28th May 2008

First published as an Advance Article on the web 18th September 2008

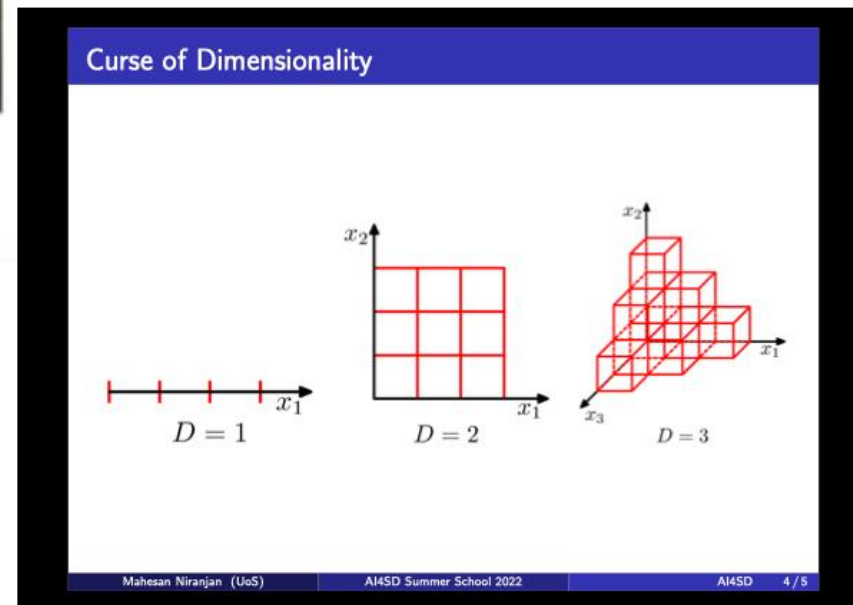
DOI: 10.1039/b805266b

# Problems

- We need for a map of chemical space
- What do we mean by related?
- What do we mean by “near”?
- In high dimensions useful ideas of distance become less well defined!
- Central Limit Theorem



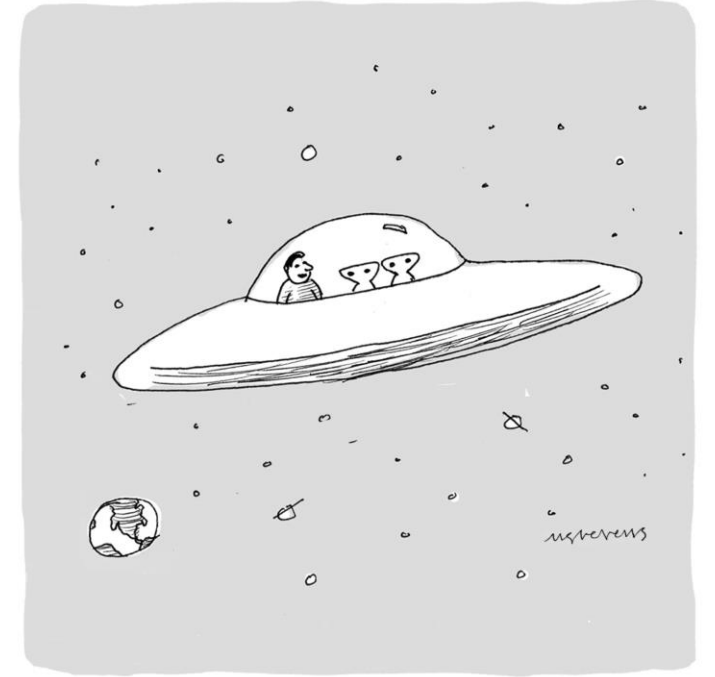
ROALD HOFFMANN



Induction  
Deduction  
Abduction

# Abduction from Molecules to Chemical Space

*How to go from the study of a few molecules to ideas about the entirety of chemical space?*

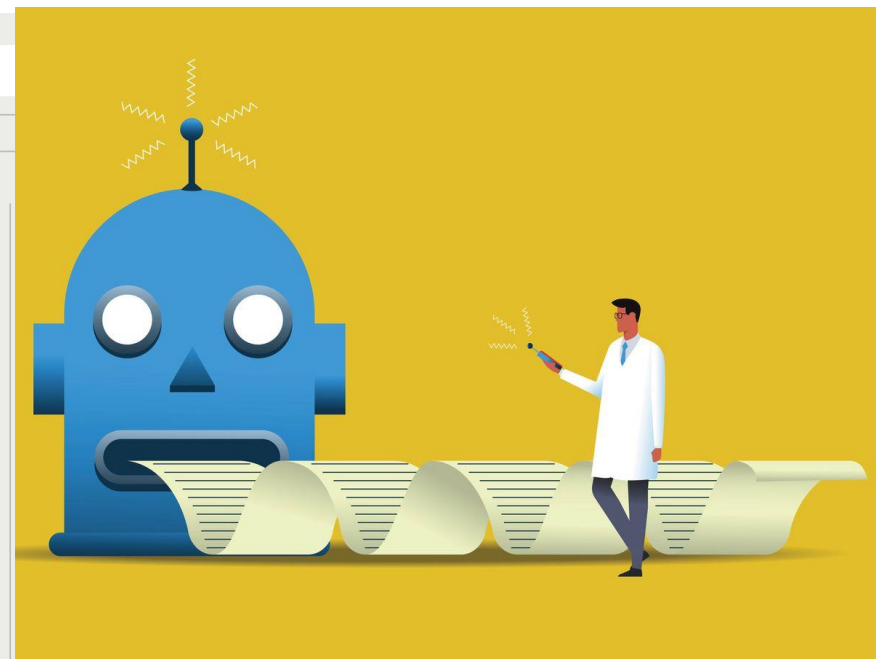


NEWS | ARTIFICIAL INTELLIGENCE

# Will the "AI Scientist" Bring Anything to Science? > A tool to take over the scientific process continues a controversial trend

BY ELIZA STRICKLAND | 09 SEP 2024 | 6 MIN READ | 📌

Eliza Strickland is a Senior Editor at IEEE Spectrum covering AI and biomedical engineering.



INTERVIEW | ARTIFICIAL INTELLIGENCE

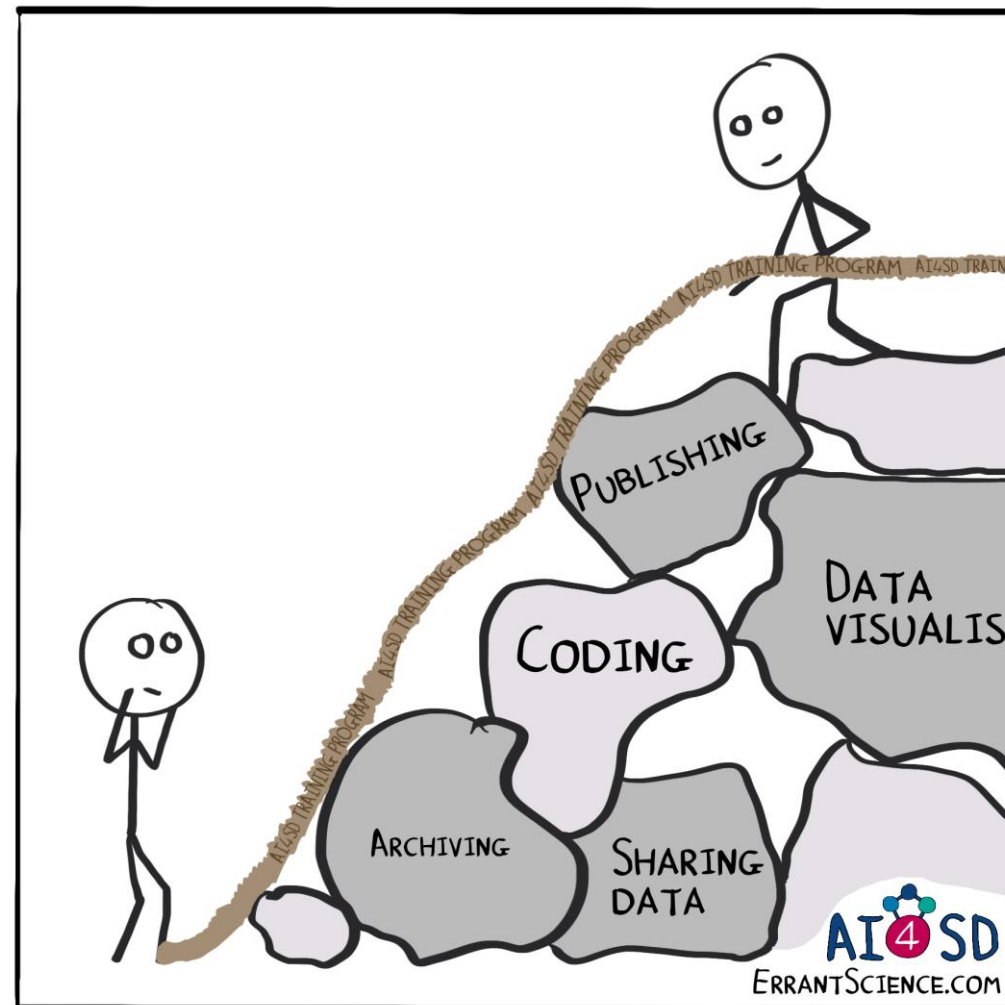
# AI Has Created a Battle Over Web Crawling > Training data may wind up in short supply as websites restrict crawler bots

BY ELIZA STRICKLAND | 31 AUG 2024 | 7 MIN READ | 📌

Eliza Strickland is a Senior Editor at IEEE Spectrum covering AI and biomedical engineering.

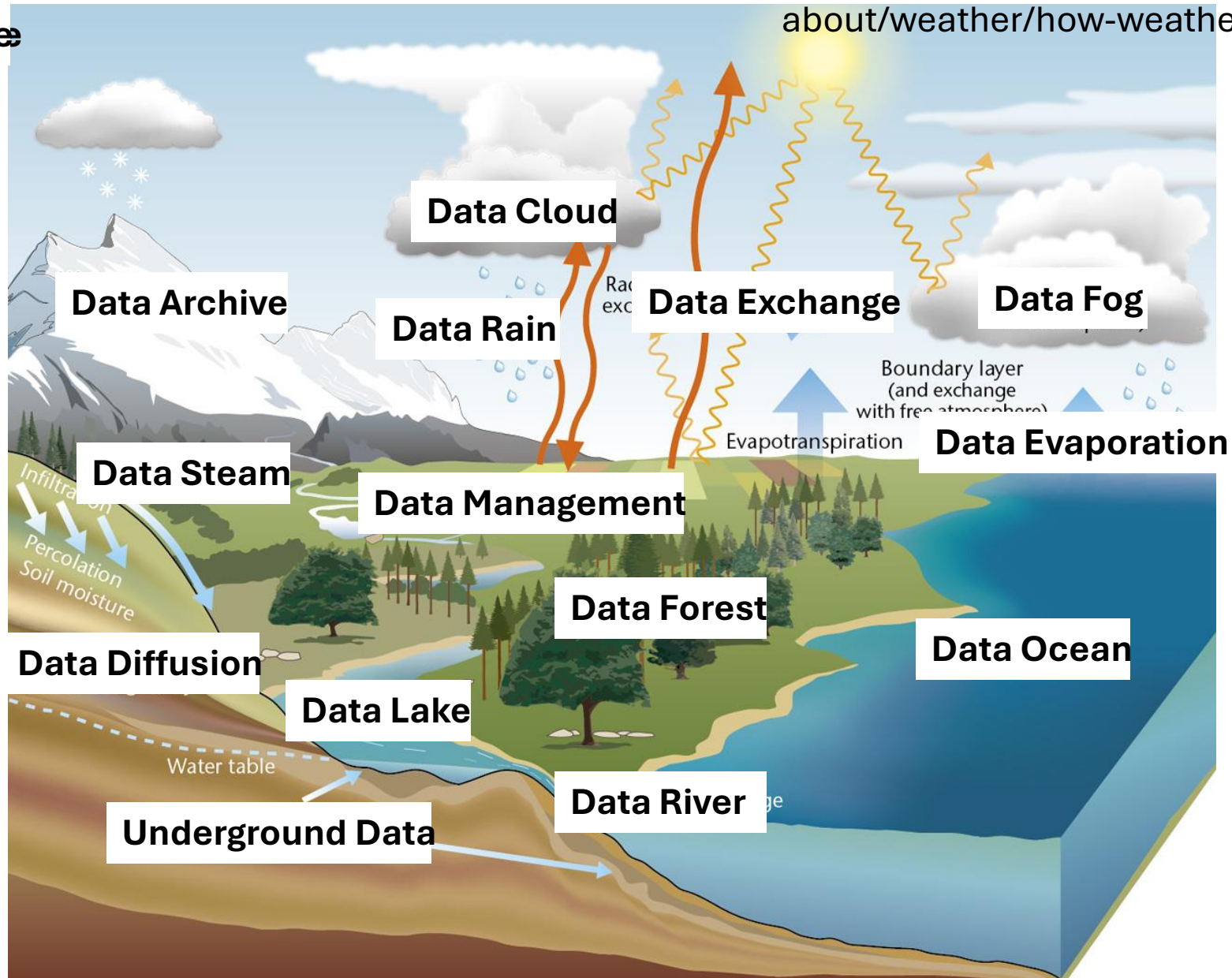


# Data

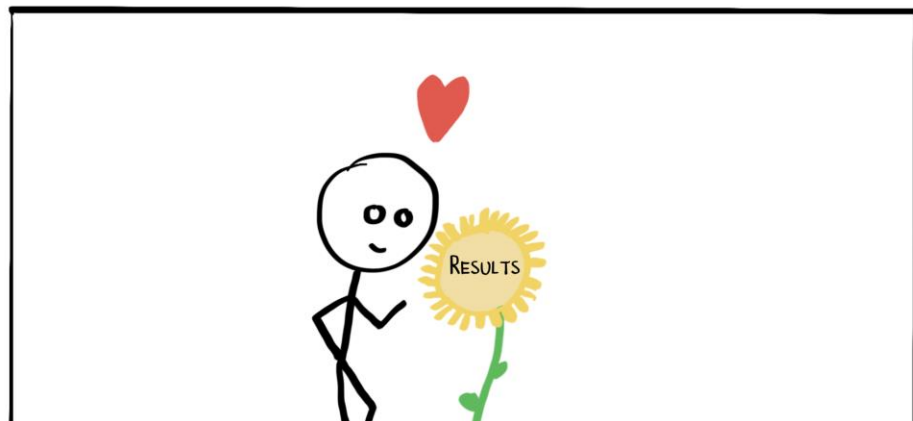


Data, data everywhere  
but not enough to model

# Data-logical Cycle



# ***Making Haystacks to find needles***



*At least get help in  
making the best  
haystack*

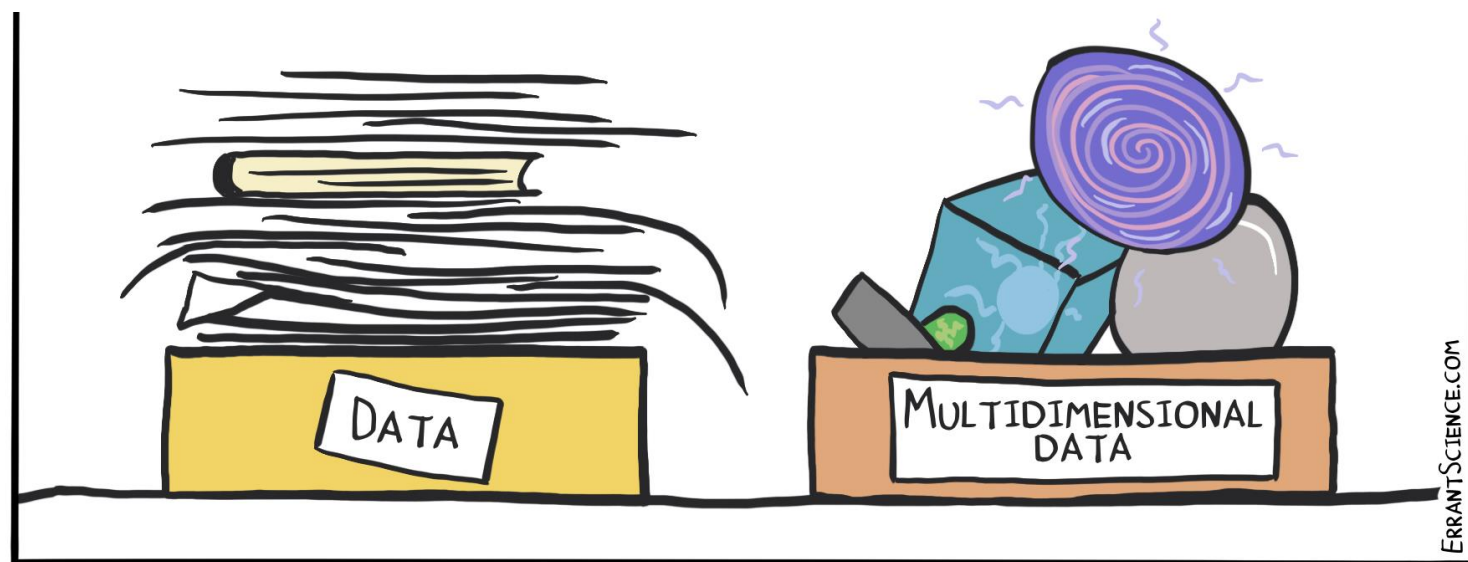
CONDITIONS





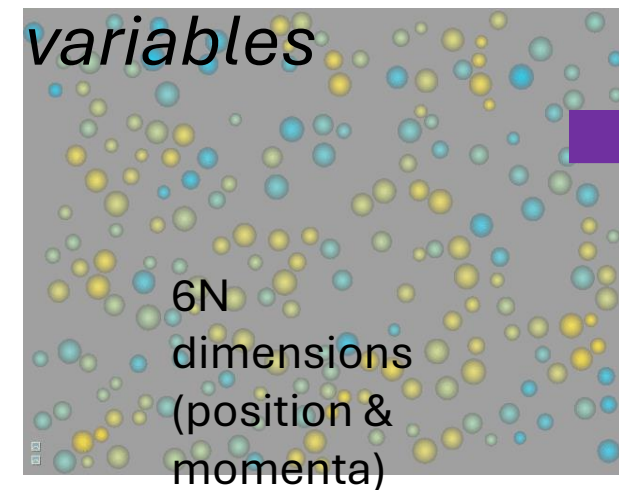
# Dimensional Reduction

25/09/2024

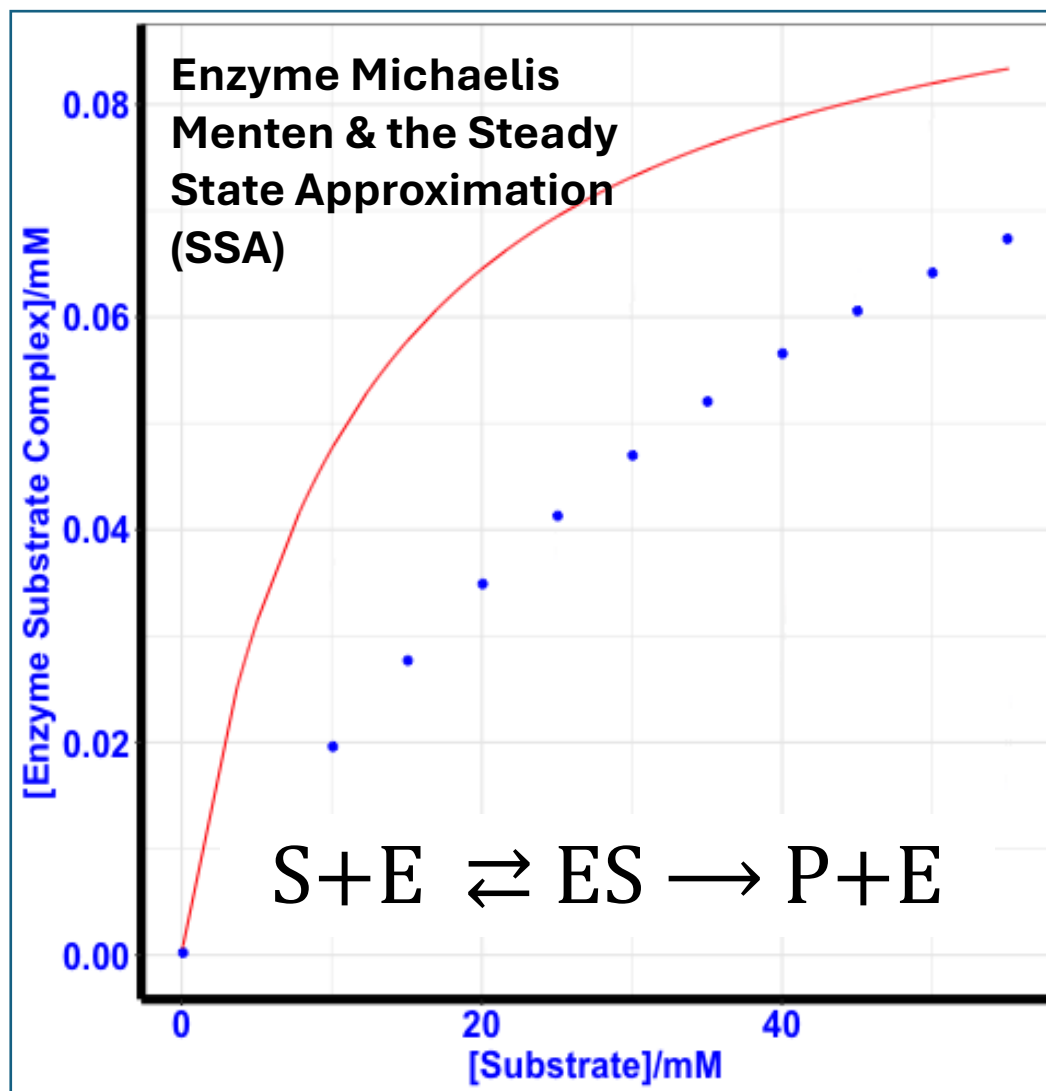
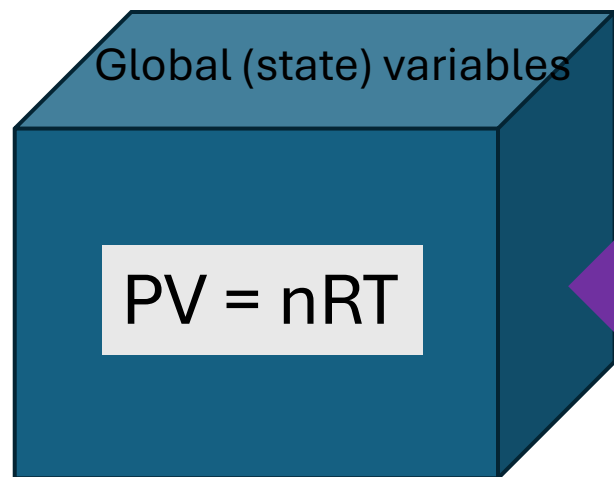




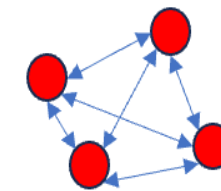
*individual particles  
to collective  
variables*



Statistical Thermodynamics

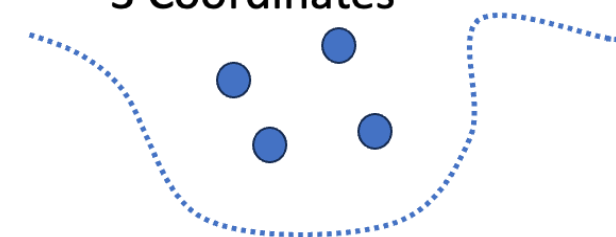


Schrodinger View  
3N Coordinates



**Formally Equivalent**

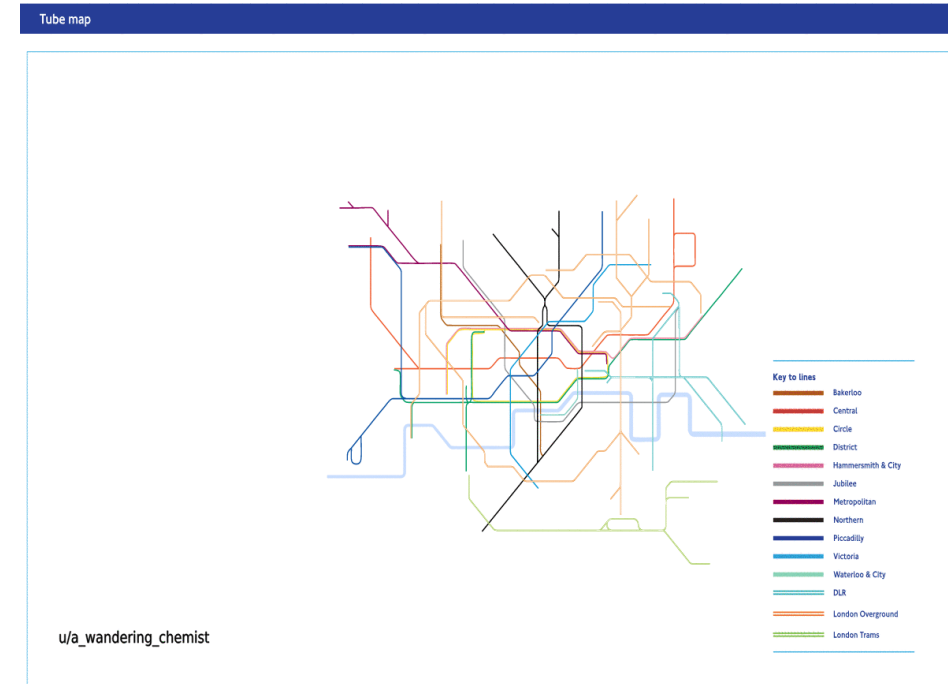
DFT View  
3 Coordinates



- Kohn-Sham particle (non-interacting)
- ..... Effective potential

# The Shape of Data – Topological Data Analysis

## Does Chemical Space have holes?



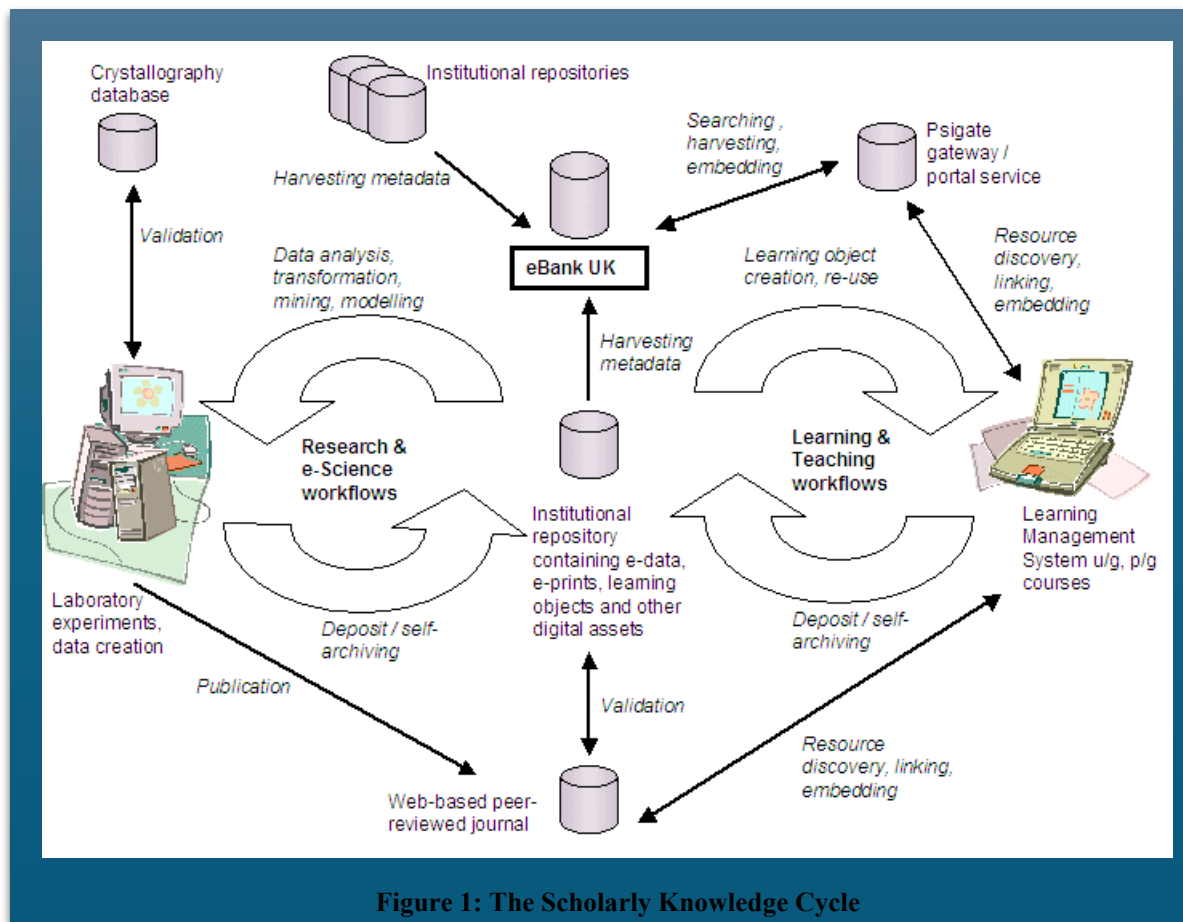
<https://pixabay.com/photos/food-eat-diet-plain-bagel-2202382/>

<https://pixabay.com/photos/oktoberfest-pretzel-meal-gastronomy-963852/>

[https://www.reddit.com/r/dataisbeautiful/comments/b8ihhr/comparison\\_between\\_the\\_london\\_tube\\_map\\_and\\_its/](https://www.reddit.com/r/dataisbeautiful/comments/b8ihhr/comparison_between_the_london_tube_map_and_its/)

At least share you haystack!

# eScience Data Infrastructures: From eBank to PSDI



PSDI  
PHYSICAL SCIENCES  
DATA INFRASTRUCTURE

Home Backgr

## Physical Sciences Data Infrastructure

An Integrated Data Infrastructure for the Physical Sciences

PSDI aims to accelerate research in the physical sciences by providing a data infrastructure that brings together and builds upon the various data systems researchers currently use.

(HTML) dc:identifier and/or "text" Subject service Searching, linking and embedding

[https://eprints.soton.ac.uk/8183/1/eBank\\_AHM.pdf](https://eprints.soton.ac.uk/8183/1/eBank_AHM.pdf)

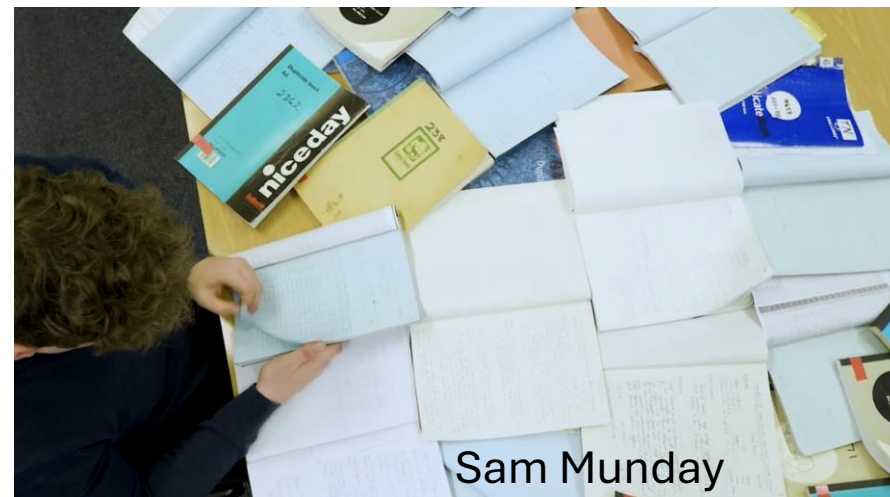
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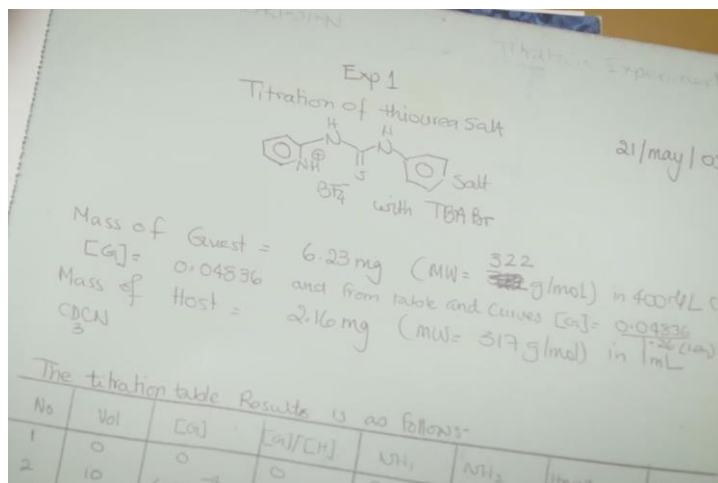
<http://www.ukoln.ac.uk/projects/ebank-uk/dissemination/PV2004-heery.pdf>

26

# DATA REVIVAL - Recover old inaccessible data

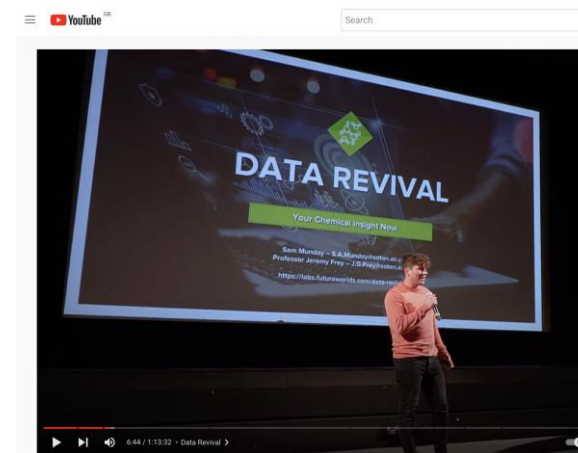


Sam Munday

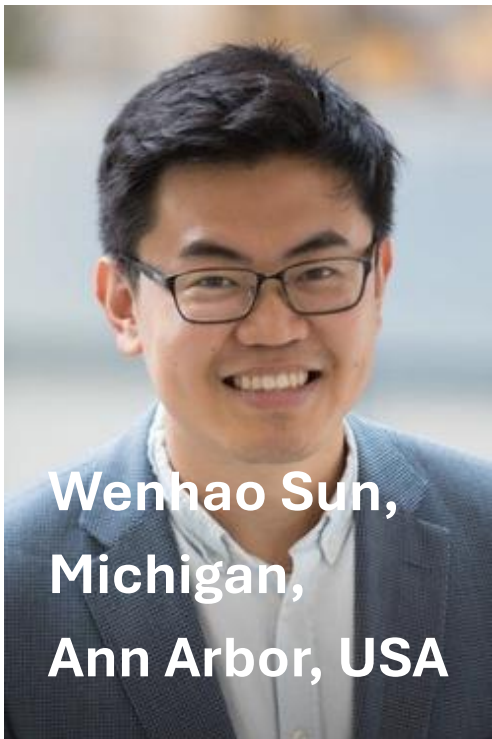


<https://www.data-revival.com>

UoS stored Chemistry  
notebooks  
~ 2000 Chemists years  
~ 10 Tb scanned data

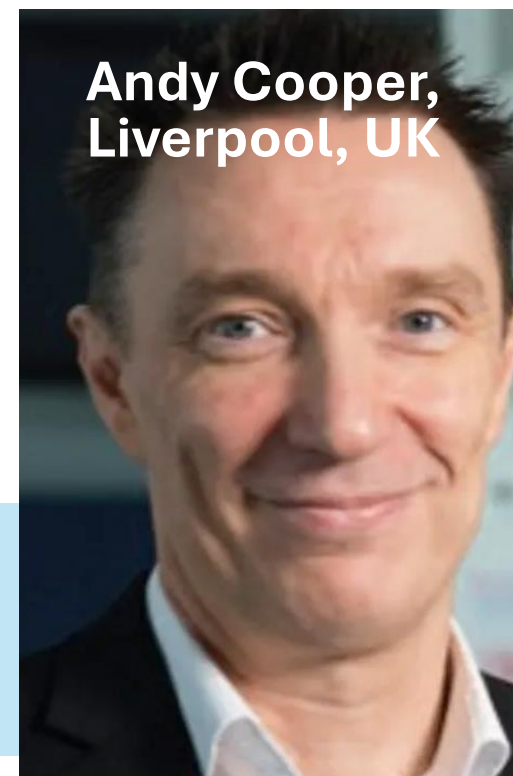


<https://www.youtube.com/watch?v=kJaICEEYHQY&t=365s>



“Extracting details of material synthesis from the literature, tells us more about what experimental researchers think about synthetic possibilities, than what is synthetically possible.”

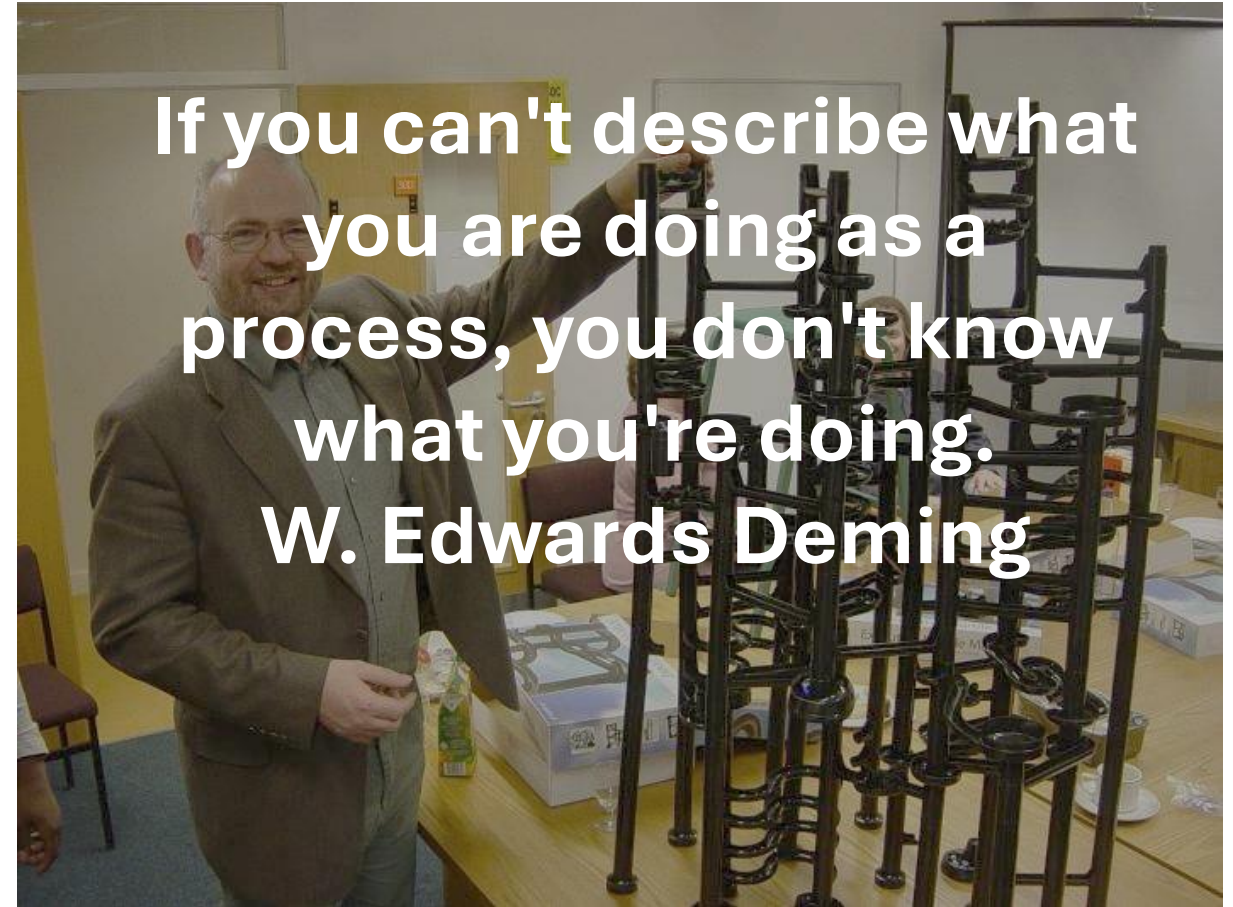
**Faraday Discussion, Data Driven Science,  
Trinity College Oxford, Sept 2024**



“What theoreticians think about how experimental researchers work, and the constraints that exist, rarely align with the realities of the laboratory”

# How do we communicate models and process?

- Surprisingly difficult to explain what a process involves
- Much of the detail is assumed to be understood and not explicitly discussed
- This is where the misunderstandings usually arise.



# Methods are as important as the data



BBC News - 'Show Your Working': What 'ClimateGate' means

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## NEWS

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Page last updated at 14:56 GMT, Tuesday, 1 December 2009

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### 'Show Your Working': What 'ClimateGate' means

**VIEWPOINT**  
Mike Hulme and Jerome Ravetz

The "ClimateGate" affair - the publication of e-mails and documents hacked or leaked from one of the world's leading climate research institutions - is being intensely debated on the web. But what does it imply for climate science? Here, Mike Hulme and Jerome Ravetz say it shows that we need a more concerted effort to explain and engage the public in understanding the processes and practices of science and scientists.

As the repercussions of [ClimateGate](#) reverberate around the virtual community of global citizens, we believe it is both important and urgent to reflect on what this moment is telling us about the practice of science in the 21st Century.



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**Reviving Rio**  
The second Earth Summit holds the promise to cure the world's environmental ills

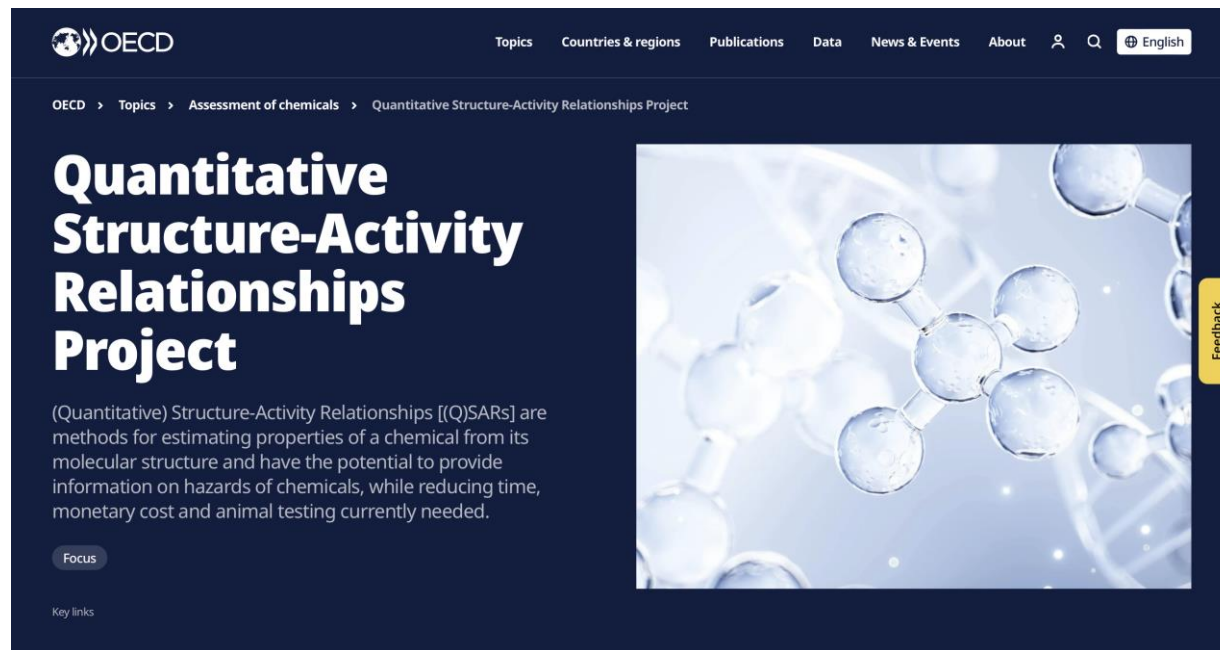
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- Hailing the arrival of alien predators
- Abduction of chemical weapons rights

# OECD Principles of QSAR (ML) Modelling .... from 2004

- Add a Principle '0' – Characterize the data
- ... the original OECD principles did not call out a specific principle to capture the importance of data aggregation and curation prior to modelling,
- Transparency in Modeling through Careful Application of OECD's QSAR/QSPR Principles via a Curated Water Solubility Data Set,
- C. N. Lowe, *et al*, Chemical Research in Toxicology 2023 36 (3), 465-478



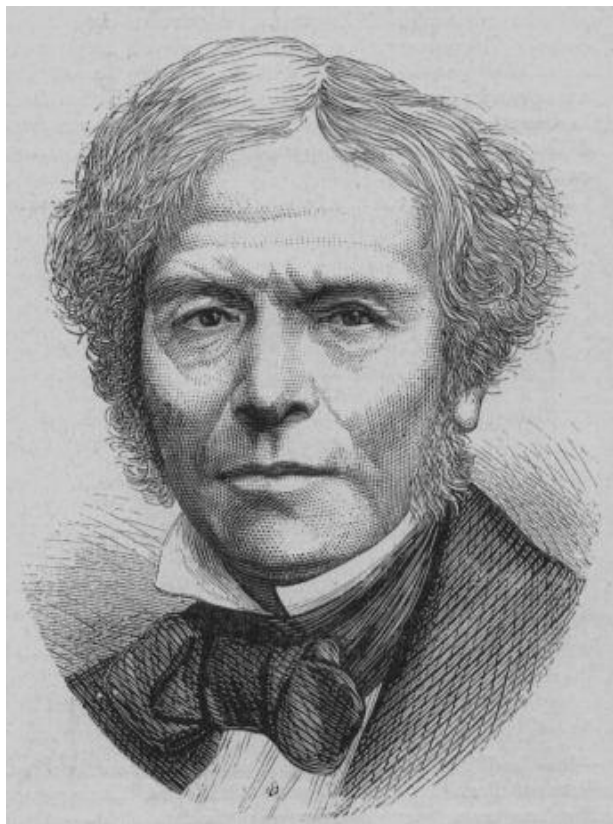
The screenshot shows the OECD website page for the Quantitative Structure-Activity Relationships Project. The page features a dark blue header with the OECD logo and navigation links: Topics, Countries & regions, Publications, Data, News & Events, About, a search icon, and a language selector set to English. Below the header, the breadcrumb trail reads: OECD > Topics > Assessment of chemicals > Quantitative Structure-Activity Relationships Project. The main content area has a large title "Quantitative Structure-Activity Relationships Project" in white text on a dark blue background. To the right of the title is a large image of a molecular structure with blue and white spheres. Below the title, a paragraph of text explains that (Quantitative) Structure-Activity Relationships [(Q)SARs] are methods for estimating properties of a chemical from its molecular structure and have the potential to provide information on hazards of chemicals, while reducing time, monetary cost and animal testing currently needed. At the bottom left of the main content area, there is a "Focus" button and a "Key links" section. A vertical "Feedback" button is located on the right side of the page.



# ON BEING A SCIENTIST

A GUIDE TO RESPONSIBLE CONDUCT IN RESEARCH

T H I R D E D I T I O N



*Faraday's laboratory notebooks are also remarkable in the amount of detail that they give about the design and setting up of experiments, interspersed with comments about their outcome and thoughts of a more philosophical kind. All are couched in plain language, with many vivid phrases of delightful spontaneity....*

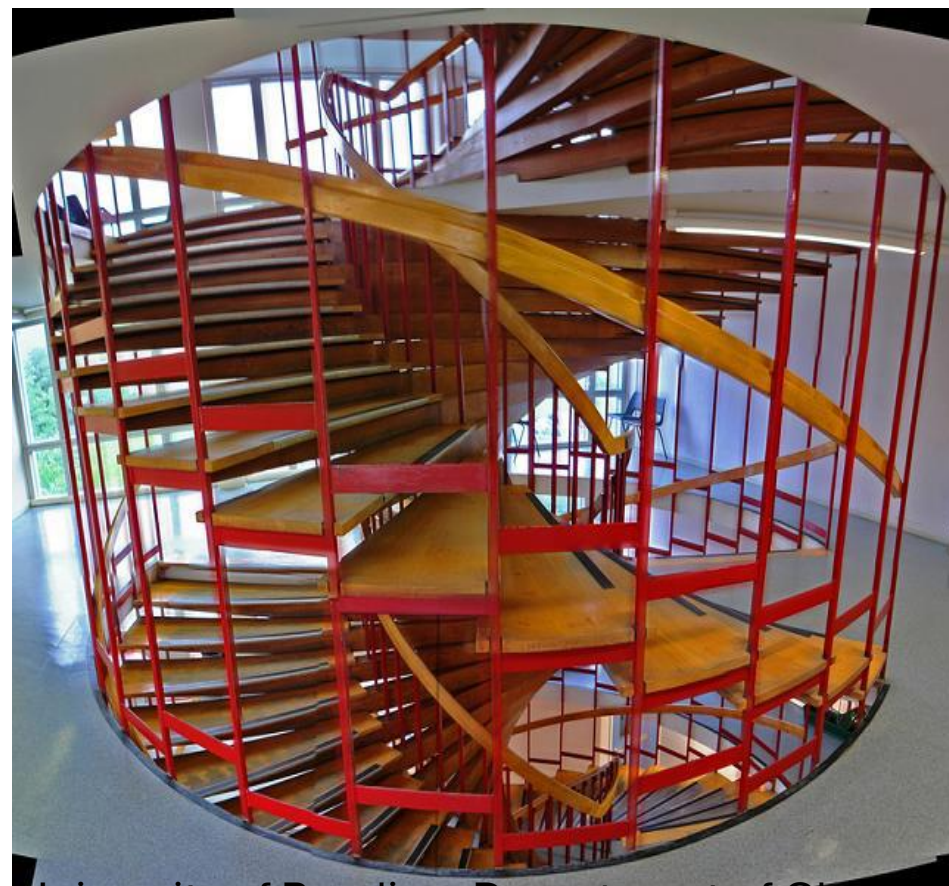
Peter Day, 'The Philosopher's Tree: A Selection of Michael Faraday's Writings'



## Welcome

Welcome to the Davy Notebooks Project website. Our site – especially the [Blog](#) section – is updated frequently. Project updates will be posted to our social media feeds ([Twitter feed](#) embedded, and buttons, below). To join the project mailing list or to send any queries to the project team, please use our [Contact](#) page.

- The aim is for the IUPAC standards to facilitate the smooth interaction of people, computers and equipment on a global scale.
- Producers and Consumers of data must not be like the non-communicating paths of a double spiral staircase (DNA)



University of Reading, Department of Chemistry

## *Chemistry is a Social Machine*

# Can Scientific Discovery Be Automated?

Progress in the sciences can only move as fast as humans can think—outsourcing to A.I. could change that.

AHMED ALKHATEEB | APR 25, 2017 | SCIENCE

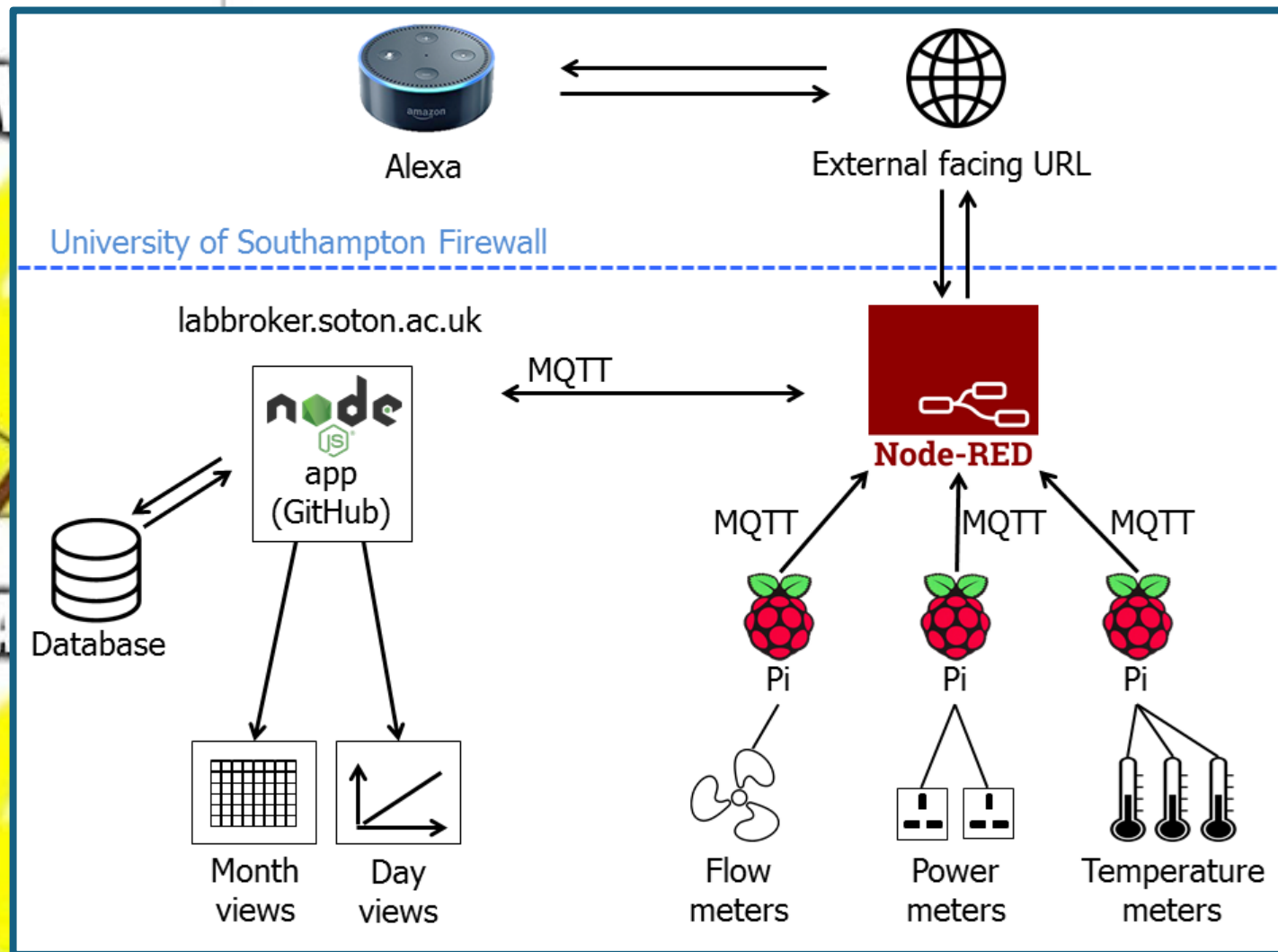
The twin challenges of too much quantity and too little quality are rooted in the finite neurological capacity of the human mind. Scientists are deriving hypotheses from a smaller and smaller fraction of our collective knowledge and consequently, more and more, asking the wrong questions, or asking ones that have already been answered. Also, human creativity seems to depend increasingly on the stochasticity of previous experiences—particular life events that allow a researcher to notice something others do not. Although chance has always been a factor in scientific discovery, it is currently playing a much larger role than it should.

# What do we need to do to get the data we want?

Augmented Intelligence

AI  
needs  
IA

Information Architecture



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Last Updated: Friday, 4 February, 2005, 08:47 GMT

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### Chemists escape labs via mobiles

By Jo Twist  
BBC News science and technology reporter

**A blend of mobile technology and award-winning software is letting scientists finally escape the lab.**

The software, called "middleware", lets different computer systems talk to each other securely and instantaneously.

As part of a national e-Science project in the UK, it is being used to let Southampton University chemists monitor experiment conditions from mobiles.

Sensors in the lab pick up any changes in the environment so the system can alert chemists, wherever they are.

"It replaces the traditional notebook with some electronic form, but it is not just about carrying around a computer - it is much smarter than that," Dr Jeremy Frey, from Southampton University, told the BBC New website.

"We wanted to be able to monitor and keep tabs on experiments outside the labs," he explained.



The system is not smart enough to actually buy a round yet

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- University of Southampton
- Combechem (e-Science project)
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- Higgs discovery rumour is denied

News feeds

# 25<sup>th</sup> Anniversary of MQTT

<http://news.bbc.co.uk/1/hi/sci/tech/4233757.stm>

It could also realise the promise of controlling home environments from phones easily and seamlessly.

But there are many other potential applications for the monitoring jobs done by the power industries, healthcare professions and other labs.



Chemists enjoy a drink at the bar while keeping an eye on the lab

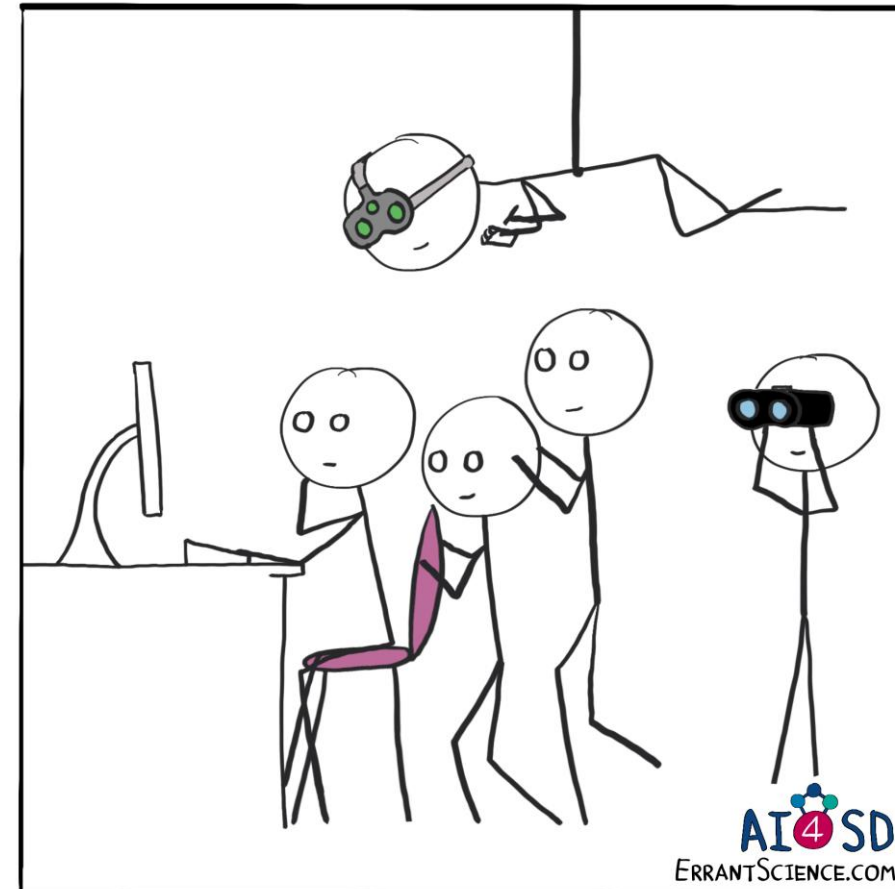
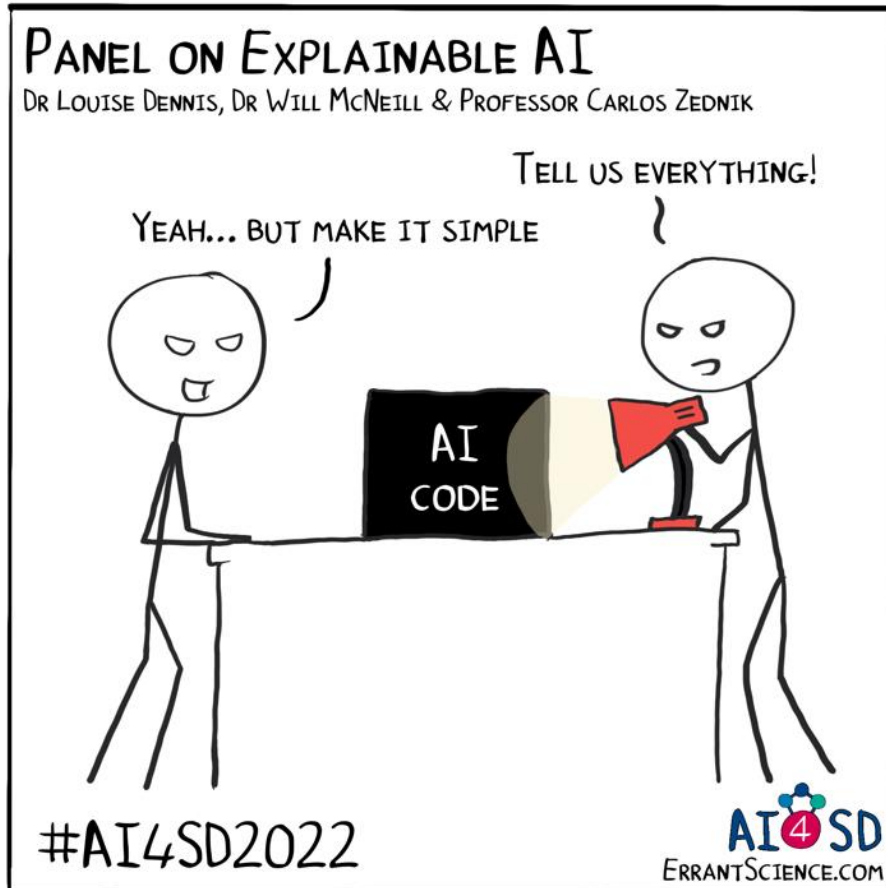
IBM won the Royal Academy of Engineering's MacRobert prize which rewards technological and engineering innovation for the program in June last year.

Used by top global banks, the WebSphere MQ family is a decade old.

It has transformed e-commerce because of its ability to allow data transfers across computer systems and different platforms without extra coding.

Friday, 4 February, 2005, 08:47 GMT

# Ethical & Explainable AI Needed for scientific discovery





Derek Lowe

## In the Pipeline Chemistry World

... Do you know who will find these things out? Not our AI and ML systems, although I'm sure they'll help whenever possible. No, it is going to be us. Just like it always has been. The law of conservation of data

Should students  
give up with  
traditional  
chemistry and  
traditional  
chemistry  
courses?

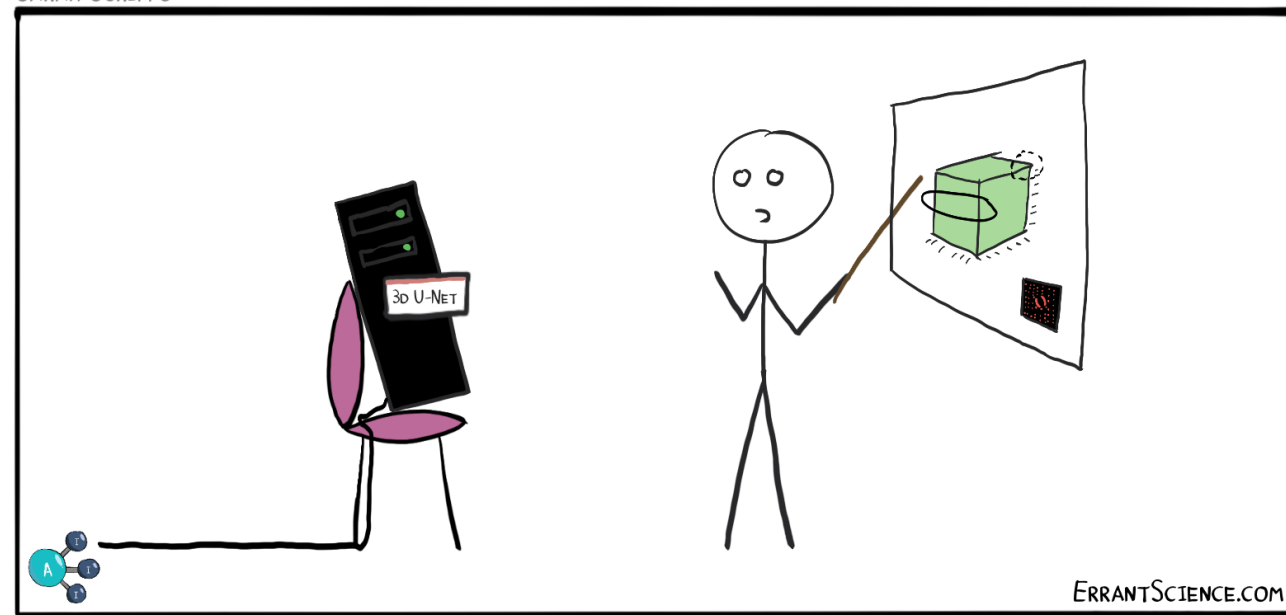
**ChatGPT  
Education  
will need  
to change!**

LEARNING THE CRYSTALLOGRAPHIC PHASE PROBLEM

SARAH SCRIPPS

#SKILLS4SCIENTISTS

#CARTOONABSTRACT



# Limits of Chemical Computation

**nature**

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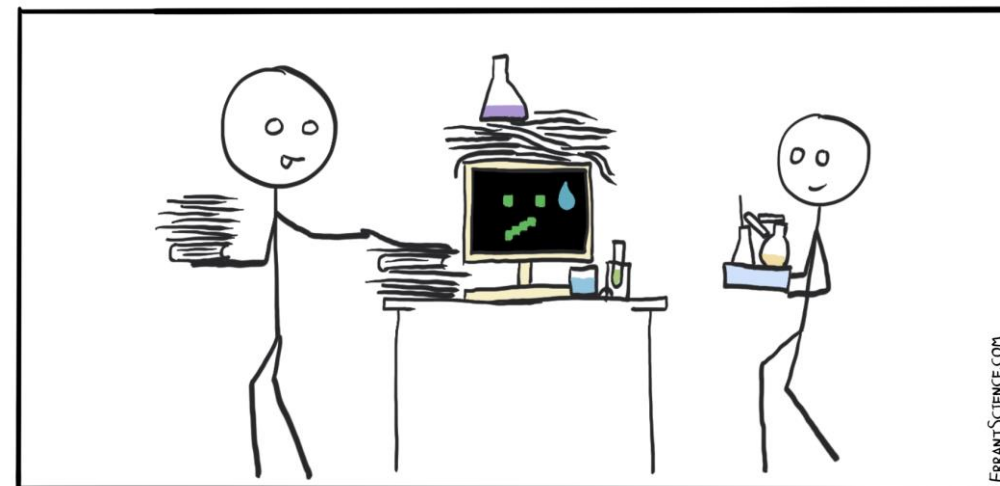
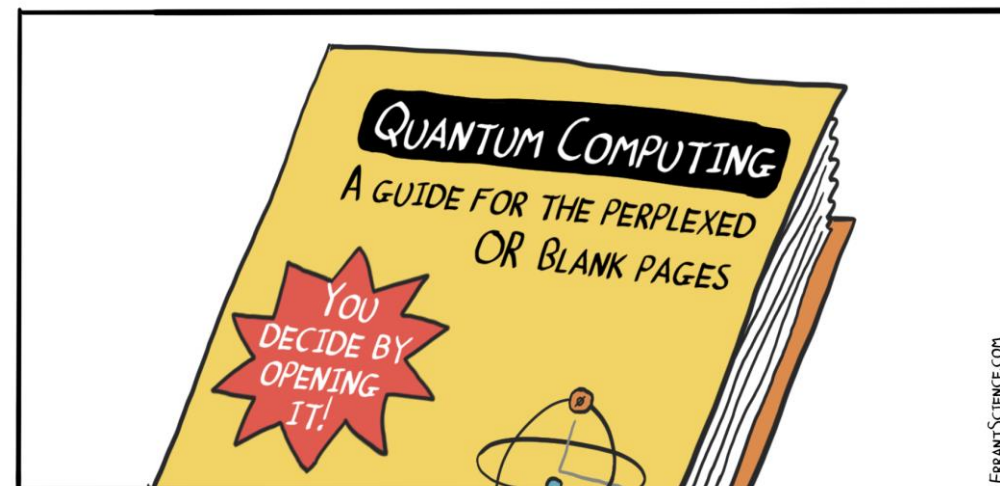
Published: 09 December 2015

## Undecidability of the spectral gap

Toby S. Cubitt [✉](#), David Perez-Garcia & Michael M. Wolf

*Nature* **528**, 207–211 (2015) | [Cite this article](#)

There are computationally undecidable problems in quantum chemistry!







# Data & Decisions

## Data

Should be FAIR

---

Findable

---

Accessible

---

Interoperable

---

Reusable

---

*Barend Mons et al 2016*

## Decisions

should be Intelligently Open

---

Accessible

---

Comprehensible

---

Useable

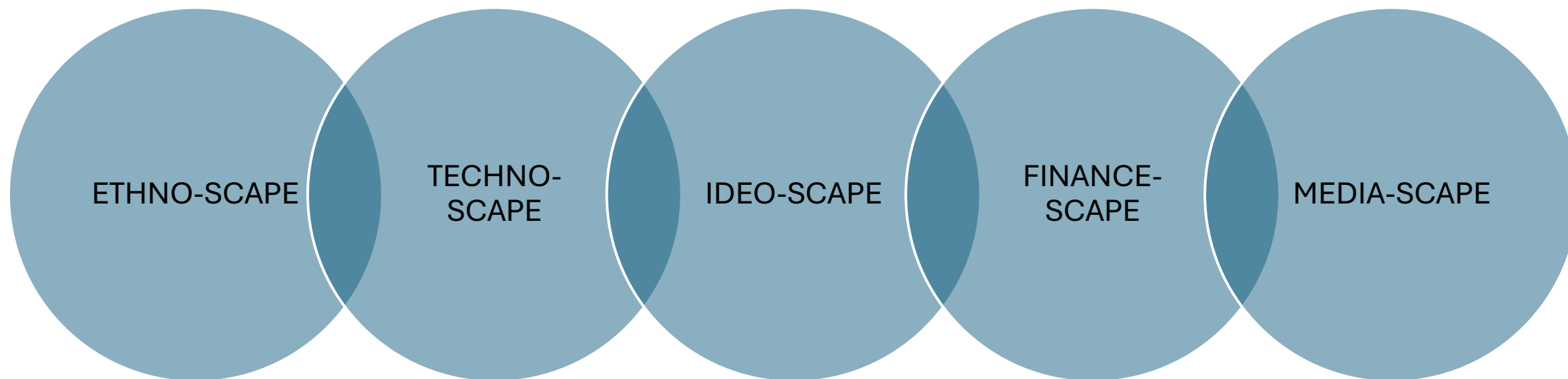
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Assessable

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*Onora O'Neil 2002*

# *Appadurai's 5-scapes for globalisation: Global (Chemical) Cultural Flow*



Chemists, Cooperation, Equipment, Society, Industry, Funding, Dissemination, Data

# Limits of Chemical Computation



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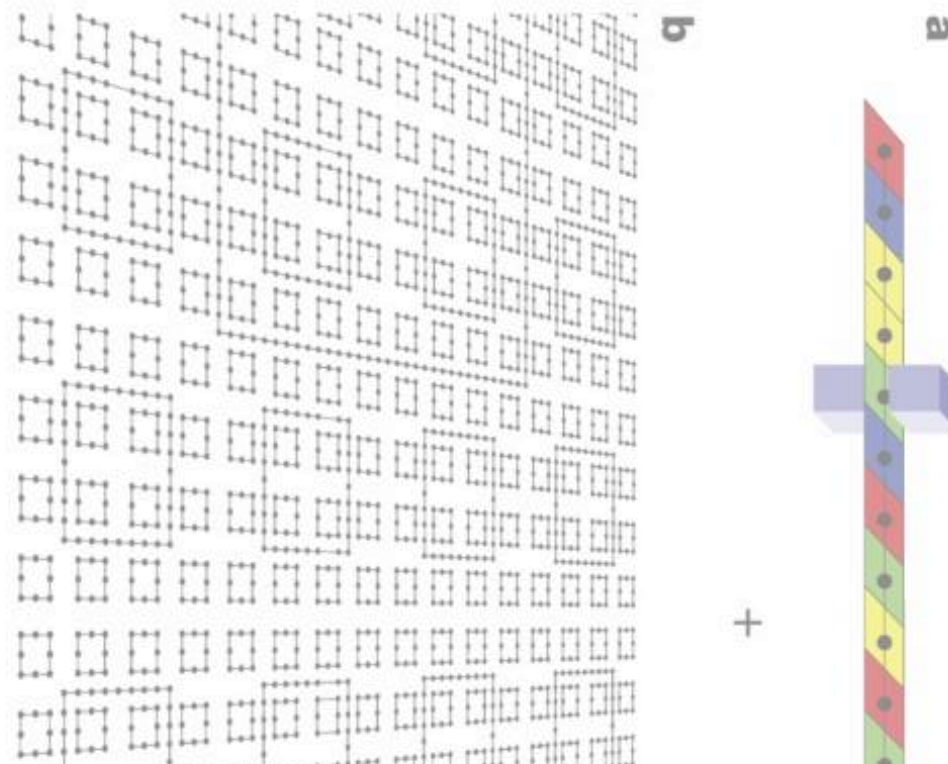
Published: 09 December 2015

### Undecidability of the spectral gap

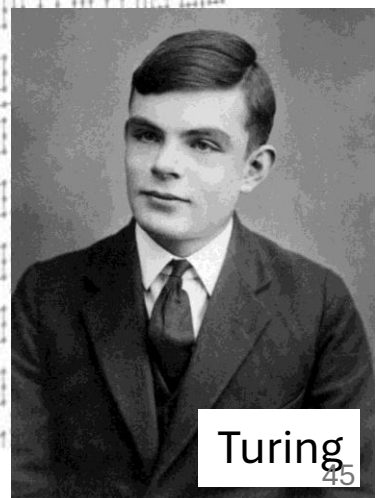
Toby S. Cubitt , David Perez-Garcia & Michael M. Wolf

Nature 528, 207–211 (2015) | Cite this article

There are computationally undecidable problems in quantum chemistry!



Gödel



Turing

# We are still in a Liminal period



# Dissemination is part of the research But beware of “Engrooved behaviour”

concept highlighted in teaching by  
Paul Trowler

<http://www.brad.ac.uk/sustainable-universities/media/sustainableuniversities/Keynote-Prof-Paul-Trowler.pdf>



<http://www.todayandtomorrow.net/2010/02/22/quarter-mile-groove/>

# The Future (is ours to see)

**When** chemistry becomes a discipline, mathematical chemists will design new materials, predict their properties, and tell engineers how to make them — without ever entering a laboratory. **We've got a long way to go on that one!**

Robert A. Heinlein, “Where to?” 1950



# Thank you for listening



and all the brilliant members of my research group and my excellent colleagues, that made this work possible



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Trust me Mort - no electronic communications superhighway, no matter how vast and sophisticated, will ever replace the art of the schmooze



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All I am saying is that now is the time to develop the technology to deflect an asteroid



**Digital chemistry:  
Paradigm shift,  
cultural evolution  
or business as usual?**

**Jeremy Frey**

University of Southampton  
Head Computational Systems Chemistry